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Ex^{2}Box: Interdependent Modes of Binding in a Two-Nanometer-Long Synthetic Receptor

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Supplementary Information

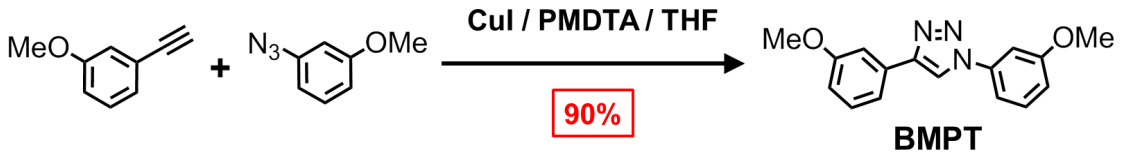
Table of Contents

Section A. Materials / General Methods / Instrumentation

All reagents were purchased from commercial suppliers and used without further purification unless stated otherwise. Solvents were deoxygenated by passing Ar through the solvent for 30 min. 1,5-Dinaphtho[38]crown-10 (DN38C10) was synthesized as previously reported.[1] Analytical high-performance liquid chromatography (HPLC) was performed on reverse-phase HPLC (RP-HPLC) instruments, using a C_{18}-column and a binary solvent system (MeCN and H_2O with 0.1% CF_3CO_2H). Thin-layer chromatography (TLC) was performed on silica gel 60 F254 (E Merck). Column chromatography was carried out on silica gel 60F (Merck 9385, 0.040–0.063 mm). UV/Vis Absorbance spectra were recorded using a UV-3600 Shimadzu spectrophotometer. Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Avance III 600 MHz, Bruker Avance III 500 MHz, and Agilent 500 MHz spectrometers, with working frequencies of 600, 500, and 500 MHz, respectively (^{1}H NMR), and 150, 125, and 125 MHz, respectively (^{13}C NMR). Chemical shifts are reported in ppm relative to the signals corresponding to the residual non-deuterated solvents (CD_3CN: δ_H = 1.94 ppm and δ_C = 1.32 and 118.26 ppm; $CDCl_3$: δ_H = 7.26 ppm and δ_C = 77.16 ppm). High-resolution mass spectra (HRMS) were measured on an Agilent 6210 Time-of-Flight (TOF) LC-MS, using an ESI source, coupled with Agilent 1100 HPLC stack, using direct infusion (0.6 mL min^{-1}). Cyclic voltammetry (CV) experiments were carried out at room temperature in argon-purged solutions in DMF with a Gamry Multipurpose instrument (Reference 600) interfaced to a PC. All CV experiments were performed using a glassy carbon working electrode (0.071 cm^2). The electrode surface was polished routinely with 0.05 μm alumina–water slurry on a felt surface immediately before use. The counter electrode was a Pt coil and the reference electrode was a Ag/AgCl electrode. The concentration of the sample and supporting electrolyte, tetrabutylammonium hexafluoro-phosphate ($TBAPF_6$), were 1.0 mM and 0.10 M, respectively. The CV cell was dried in an oven immediately before use and argon was flushed continually through the cell as it was cooled down to room temperature to avoid condensation of water.

B. Synthetic Protocols

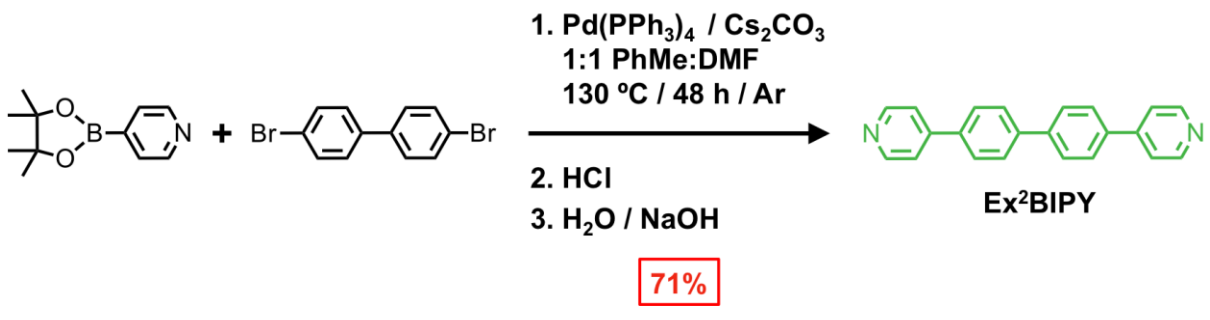
1) 1,4-Bis(3-methoxyphenyl)-1H-1,2,3-triazole – "BMPT"



Scheme S1. Synthesis of 1,4-bis(3-methoxyphenyl)-1*H*-1,2,3-triazole – **BMPT**.

BMPT: A mixture of 3-ethynylanisole (0.38 g, 2.9 mmol), 3-azidoanisole (0.43 g, 2.9 mmol), CuI (55 mg, 0.29 mmol), *N*,*N*,*N*',*N*',*N*''-pentamethyldiethylenetriamine (PMDTA, 50 mg, 0.29 mmol), and deoxygenated THF (30 mL) was stirred at room temperature under Ar for 24 h. The crude reaction mixture was concentrated *in vacuo* and subjected to column chromatography using silica gel and CH_2Cl_2, yielding pure product (0.74 g, 91%) as a pale yellow oil. HRMS-ESI for **BMPT**; Calcd for $C_{16}H_{15}N_3O_2$: *m/z* = 282.1237 $[M + H]^+$; Found: 282.1242 $[M + H]^+$. ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ_H 8.17 (s, 1H), 7.53 (dd, *J* = 2.7, 1.5, 1H), 7.46–7.42 (m, 2H), 7.40 (dd, *J* = 2.3, 2.3 Hz, 1H), 7.37 (dd, *J* = 7.9, 7.9 Hz, 1H), 7.32 (ddd, *J* = 7.6, 1.9, 0.7 Hz, 1H), 6.99 (ddd, *J* = 8.0, 2.4, 0.7 Hz, 1H), 6.94–6.91 (ddd, *J* = 8.3, 2.6, 1.0 Hz, 1H), 3.91 (s, 3H), 3.90 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ_C 160.6, 160.1, 148.2, 138.1, 131.5, 130.6, 130.0, 118.2, 117.9, 114.7, 114.5, 112.4, 110.9, 106.4, 55.7, 55.4.

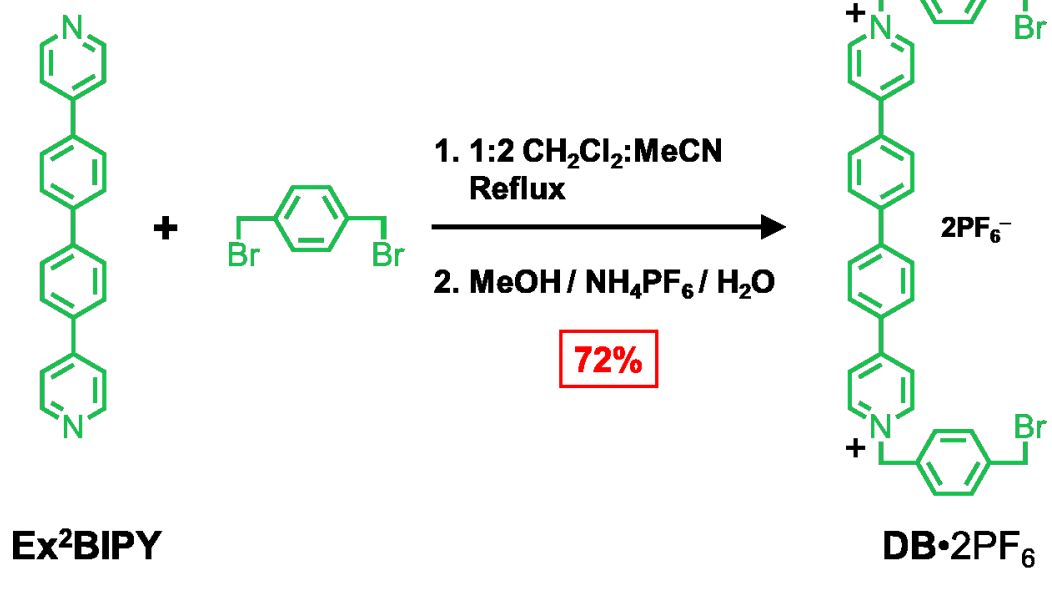
2) 4,4'-(4,4'-Biphenylene)bipyridine – "Extended Bipyridine = Ex^{2}BIPY"



Scheme S2. Synthesis of 4,4′-(4,4′-biphenylene)bipyridine – **Ex^{2}BIPY**.

Ex^{2}BIPY: A mixture of pyridin-4-ylboronic acid pinacol ester (10.0 g, 48.8 mmol), 4,4′-dibromo-1,1′-biphenyl (6.09 g, 19.5 mmol), $Pd(PPh_3)_4$ (1.13 g, 0.970 mmol), Cs_2CO_3 (22.6 g, 117 mmol), and a 1:1 mixture of dry PhMe/DMF (500 mL) was heated to 130 ºC under Ar for 72 h before the hot reaction mixture was rendered acidic (pH 2–3) by adding dropwise concentrated HCl, which caused the crude product to precipitate from solution. Then, the reaction mixture was cooled to room temperature, filtered, and washed with CH_2Cl_2. The solid was dispersed in H_2O at 80 ºC and the insoluble material was filtered off before an aqueous NaOH solution (10 M) was added dropwise to the filtrate until the pH was ~8–9, resulting in precipitation of the desired product. The solid was filtered and washed with H_2O, dissolved in a 1:1 mixture of hot $CHCl_3$/PhMe, and filtered through Celite. The filtrate was concentrated *in vacuo*, yielding pure **Ex^{2}BIPY** (4.2 g, 71%) as a white solid. HRMS-ESI for **Ex^{2}BIPY**; Calcd for $C_{22}H_{16}N_2$: m/z = 309.1386 $[M + H]^+$; Found: 309.1383 $[M + H]^+$. ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ_H 8.70 (AA' of AA'XX', J = 6.1, 1.6 Hz, 4H), 7.83–7.78 (AA'BB', 8H), 7.57 (XX' of AA'XX', J = 6.2, 1.6 Hz, 4H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ_C 150.5, 147.8, 141.1, 137.6, 127.9, 127.7, 121.6.

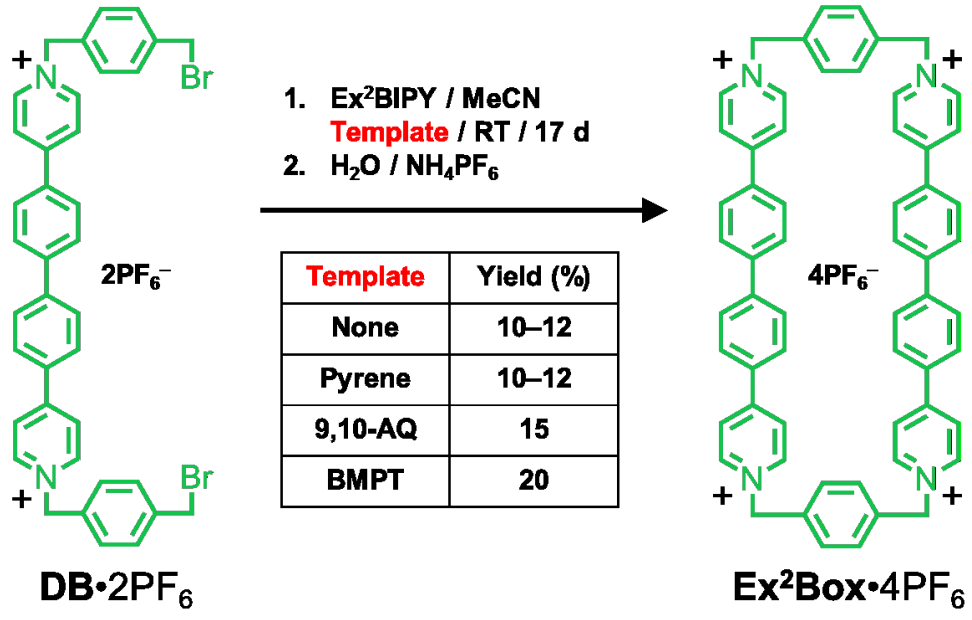
3) Bis(4-bromomethylbenzyl)(4,4'-(4,4'-biphenylene)bipyridin-1-ium)bis(hexafluoro-phosphate) = "DB•2PF$_6$"



Scheme S2. Synthesis of **DB**•2PF$_6$.

DB•2PF$_6$: α,α'-Dibromo-*p*-xylene (5.14 g, 19.5 mmol) was added to a 1:1 mixture of CH_2Cl_2/MeCN (240 mL) in a round-bottomed three-necked flask and the resulting mixture was heated at 50 ºC while stirring until all of the solid material dissolved. Next, the temperature of the oil bath was raised to 90 ºC and a suspension of **Ex^{2}BIPY** (600 mg, 1.95 mmol) in MeCN (120 mL) was added in four aliquots slowly over the course of 4 h. After heating under reflux for 24 h, the reaction mixture was cooled to room temperature and the yellow precipitate was collected by filtration and washed with CH_2Cl_2. The yellow solid was dissolved in cold (≤RT) MeOH (~1 L) followed by the addition of NH_4PF_6 (~400 mg) and cold (≤RT) H_2O (~1 L), resulting in the precipitation of pure **DB**•2PF$_6$ (1.35 g, 72%) that was collected by filtration as a yellowish solid. HRMS-ESI for **DB**•2PF$_6$; Calcd for $C_{38}H_{31}Br_2F_{12}N_2P_2$: *m/z* = 821.0552 [*M* – PF$_6$]$^+$; Found: 821.0551 [*M* – PF$_6$]$^+$. ^{1}H NMR (500 MHz, CD_3CN, ppm): δ_H 8.76 (AA' of AA'XX', *J* = 6.3 Hz, 4H), 8.33 (XX' of AA'XX', *J* = 6.3 Hz, 4H), 8.07 (AA' of AA'BB', *J* = 8.2 Hz, 4H), 8.01 (BB' of AA'BB', *J* = 8.1 Hz, 4H), 7.55 (AA' of AA'BB', *J* = 7.9 Hz, 4H), 7.46 (BB' of AA'BB', *J* = 7.8 Hz, 4H), 5.70 (s, 4H), 4.61 (s, 4H). ^{13}C NMR (125 MHz, CD_3CN, ppm): δ_C 156.9, 145.3, 143.8, 141.1, 134.5, 134.3, 131.1, 130.3, 129.9, 129.3, 126.2, 64.1, 33.5.

4) Cyclobis(4,4'-(4,4'-biphenylene)bipyridin-1-ium-1,4-phenylenebis(methylene))tetrakis-(hexafluorophosphate) – "Extended Viologen Box = Ex^{2}Box•4PF$_6$"



Template	Yield (%)
None	10–12
Pyrene	10–12
9,10-AQ	15
BMPT	20

Scheme S3. Synthesis of **Ex^{2}Box**•4PF$_6$ by using various templates.

Ex^{2}Box•4PF$_6$: A representative procedure is described in detailed here. A solution of **DB**•2PF$_6$ (600 mg, 0.621 mmol), **Ex^{2}BIPY** (192 mg, 0.621 mmol), and the template pyrene (754 mg, 3.73 mmol) in dry MeCN (450 mL) was stirred at room temperature for 17 d. The reaction was quenched by adding concentrated HCl (2–3 mL), causing the crude product to precipitate from solution. The yellowish precipitate was collected by filtration and dissolved in hot MeOH. The crude **Ex^{2}Box**•4PF$_6$ was precipitated from the MeOH solution by adding NH_4PF_6 (~0.5 g) and an excess of H_2O, and was collected, before being subjected to column chromatography using silica gel and CH_2Cl_2/MeCN (1:1) and 0.25–0.5% NH_4PF_6 in MeCN (w/v) as the eluents. Recrystallization in MeCN on slow vapor diffusion of *i*Pr$_2$O yielded pure **Ex^{2}Box**•4PF$_6$ (87–104 mg, 10–12%) as a pale yellow solid. HRMS-ESI for **Ex^{2}Box**•4PF$_6$; Calcd for $C_{60}H_{48}F_{24}N_4P_4$: *m/z* = 1259.2799 $[M - PF_6]^+$, 557.1576 $[M - 2PF_6]^{2+}$; Found: 1259.2792 $[M - PF_6]^+$, 557.1590 $[M - 2PF_6]^{2+}$. ^{1}H NMR (500 MHz, CD_3CN, ppm): δ_H 8.74 (AA' of AA'XX', J = 7.0 Hz, 8H), 8.18 (XX' of AA'XX', J = 6.9 Hz, 8H), 7.89 (AA' of AA'BB', J = 8.6 Hz, 8H), 7.84 (BB' of AA'BB', J = 8.6 Hz, 8H), 7.63 (s, 8H), 5.67 (s, 8H). ^{13}C NMR (125 MHz, CD_3CN, ppm): δ_C 156.4, 144.8, 143.4, 137.0, 133.9, 131.0, 129.6, 129.1, 126.0, 64.5.

Section C. Computational Protocol

The geometries were optimized in Poisson–Boltzmann solvation model[2] for MeCN (ε = 37.5 and R_0 = 2.18 Å) at the level of M06-2x/6-311G with Jaguar 7.5.[3] The scans for the guest moving in the **Ex^{2}Box^{4+}** were carried out by fixing the relative shift between the center of **Ex^{2}Box^{4+}**, which was defined as the average of four methylene carbons of **Ex^{2}Box^{4+}**, and the center of guest, which was defined as the average of C(9) and C(10) of anthracene, 9,10-anthraquinone, and 1,4-anthraquinone. The binding energy of **Ex^{2}Box^{4+}**⊂guest complex was corrected by deducting the cost to remove four MeCN solvent molecules from the cavity of **Ex^{2}Box^{4+}**, that is, 11.1 kcal mol^{-1}.

Section D. Crystallographic Characterization

All crystallographic data are available free of charge from the Cambridge Crystallographic Data Centre (CCDC) via www.ccdc.cam.ac.uk/data_request/cif.

1) Ex²Box•4PF₆

a) Method. **Ex²Box**•4PF_6 (3.4 mg, 2.4 μmol) was dissolved in MeCN (0.8 mL) and the mixture was passed through a 0.45-μm filter equally into three 1-mL tubes. The tubes were placed together in one 20-mL vial containing *i*Pr_2O (~3 mL) and the vial was capped. Slow vapor diffusion of *i*Pr_2O into the solution of **Ex²Box**•4PF_6 in MeCN (3.0 mM) over the course of one week yielded colorless single crystals of **Ex²Box**•4PF_6. Data were collected at 100 K on a Bruker Kappa APEX2 CCD Diffractometer equipped with a CuK_α microsource with Quazar optics. The solid-state structure of **Ex²Box**$^{4+}$ is shown in Figure S1.

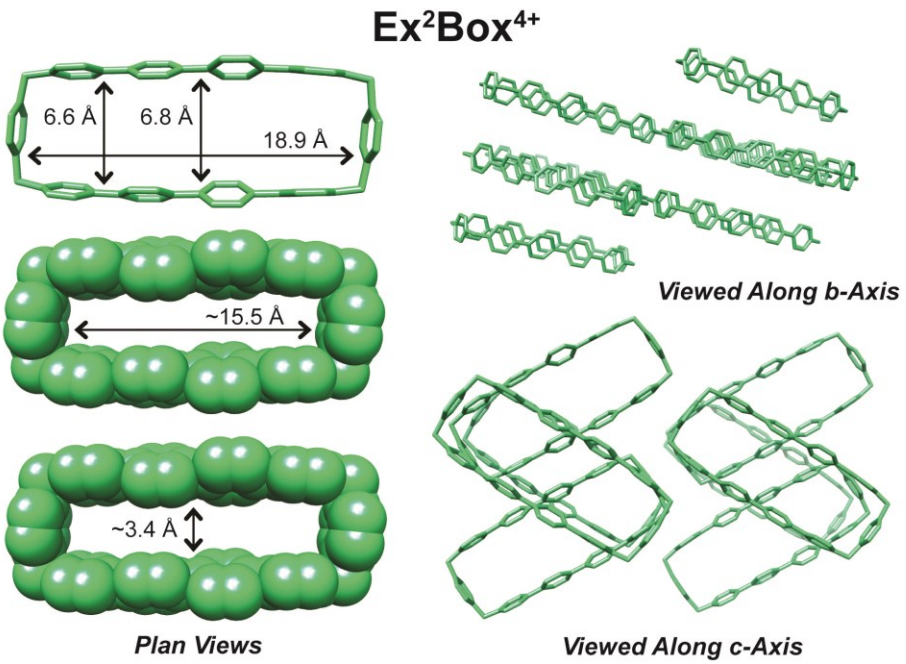


Figure S1. Different crystallographic views of **Ex²Box**$^{4+}$. Counterions and solvent molecules are omitted for the sake of clarity.

b) Crystal Parameters. $[C_{60}H_{48}N_4•(PF_6)_4]•(MeCN)_2$. Colorless block (0.18 × 0.70 × 0.04 mm). Monoclinic, $P2_1/c$, a = 20.278(8), b = 12.043(5), c = 14.511(7) Å, α = 90.000, β = 108.579(3), γ = 90.000º, V = 3358.9(3) Å^3, Z = 2, T = 100.01 K, ρ_{calc} = 1.470 g cm^{-3}, μ = 2.042 mm^{-1}. Of a total of 5570 reflections that were collected, 5570 were unique. Final R_1 = 0.0452 and wR_2 = 0.1093. Refined as a two-component twin. The crystal under investigation was found to be non-merohedrally twinned. The orientation matrices for the two components were identified using the program Cell Now[4] and the data were processed using both orientation matrices with SAINT.

The exact twin matrix identified by the integration program was found to be –0.99975 –0.00027 0.00057 / 0.00013 –1.00000 –0.00012 / 0.89137 –0.00018 0.99975. The second domain is rotated from the first domain by 180° about the reciprocal lattice *c*-axis (non-standard setting). The absorption correction was carried out using TWINABS V2008/4[5] to create an hklf5 file, which was used in all refinements; the structure was solved using direct methods with only the non-overlapping reflections of component 1. The twin fraction refined to a value of 0.4162(15). CCDC Number: 913422.

2) $Ex^2Box\subset(Anthracene)_{0.5}\bullet 4PF_6(Anthracene)$

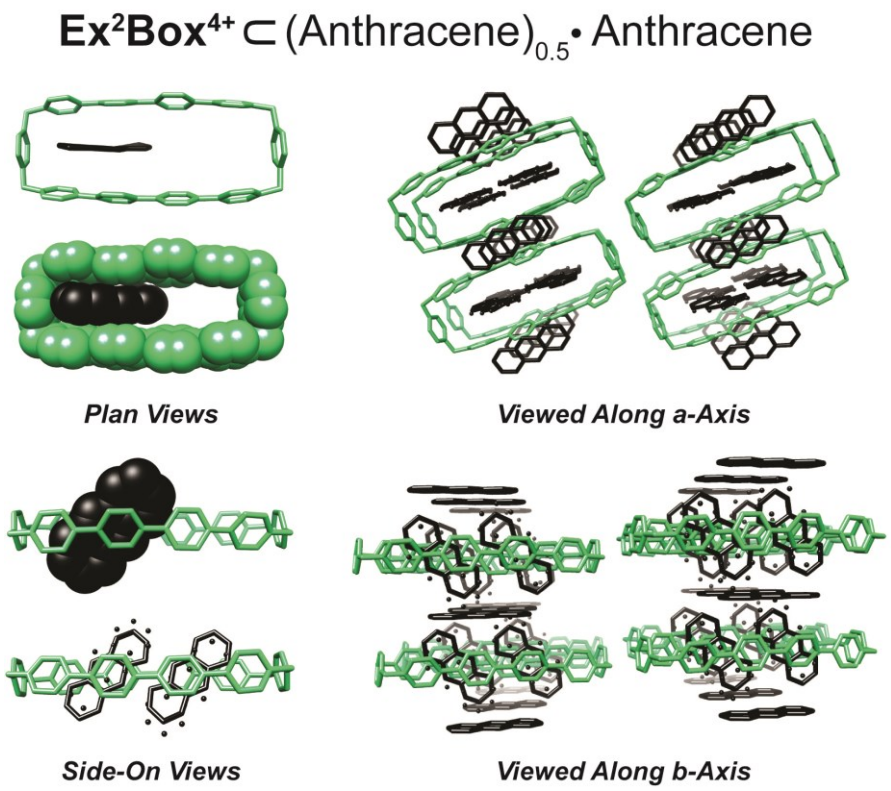


Figure S2. Different crystallographic views of $\mathbf{Ex^2Box^{4+}}\subset(anthracene)_{0.5}\bullet(anthracene)$. Half of the $\mathbf{Ex^2Box^{4+}}$ cyclophanes are occupied with one anthracene molecule and half of the $\mathbf{Ex^2Box^{4+}}$cyclophanes are empty. Anthracene molecules are disordered and each molecule of anthracene can be positioned in four different ways within $\mathbf{Ex^2Box^{4+}}$ cyclophane (bottom-left). Counterions and solvent molecules are omitted for the sake of clarity.

a) Method A. Solid anthracene (0.70 mg, 3.9 μmol) was added to a solution of $\mathbf{Ex^2Box}\bullet 4PF_6$ (3.3 mg, 2.3 μmol) in MeCN (0.8 mL) and, after it dissolved, the mixture was passed through a 0.45-μm filter equally into three 1-mL tubes. The tubes were placed together in one 20-mL vial

containing *i*Pr_2O (~3 mL) and the vial was capped. Slow vapor diffusion of *i*Pr_2O into the 2:1 solution of anthracene and **Ex^{2}Box**•$4PF_6$ in MeCN over the period of 4 d yielded yellow single crystals of **Ex^{2}Box**⊂$(anthracene)_{0.5}$•$4PF_6$(anthracene). Note the structural formula in the *Crystal Parameters* section below reflects an occupancy of only half of the **Ex^{2}Box**•$4PF_6$ cyclophanes with anthracene molecules. Data were collected at 100 K on a Bruker Kappa APEX2 CCD Diffractometer equipped with a CuK_α microsource with MX optics. The solid-state superstructure of **Ex^{2}Box^{4+}**⊂$(anthracene)_{0.5}$•(anthracene) obtained with this method is shown in Figure S2.

Method B. A solution of anthracene (2.0 mg, 11 μmol) in $CHCl_3$ (0.3 mL) was added to a solution of **Ex^{2}Box**•$4PF_6$ (2.0 mg, 1.4 μmol) in MeCN (0.8 mL) and the mixture was passed through a 0.45-μm filter equally into three 1-mL tubes. The tubes were placed together in one 20-mL vial containing *i*Pr_2O (~3 mL) and the vial was capped. Slow vapor diffusion of *i*Pr_2O into the 8:1 solution of anthracene and **Ex^{2}Box**•$4PF_6$ in MeCN over the period of 4 d yielded yellow single crystals of **Ex^{2}Box**⊂$(anthracene)_{0.5}$•$4PF_6$(anthracene). Data were collected at 100 K on a Bruker Kappa APEX2 CCD Diffractometer using a CuK_α microsource with MX optics. The solid-state superstructure was identical to that observed by *Method A*.

b) Crystal Parameters. $[C_{60}H_{48}N_4⊂(C_{14}H_{10})_{0.5}•(PF_6)_4]•(C_{14}H_{10})•(MeCN)_2$. Yellow block (0.25 × 0.10 × 0.05 mm). Triclinic, $P\bar{1}$, a = 10.061(3), b = 11.220(4), c = 21.754(7) Å, α = 77.931(18), β = 85.603(18), γ = 65.560(16)º, V = 2186.1(13) Å^3, Z = 1, T = 100.03 K, ρ_{calc} = 1.333 g cm^{-3}, μ = 0.184 mm^{-1}. Of a total of 59360 reflections that were collected, 12946 were unique (R_{int} = 0.0376). Final R_1 = 0.0898 and wR_2 = 0.2662. Distance restraints were refined for the disordered anthracene. A group anistropic displacement parameter was refined for the disordered anthracene, which was also restrained (esd 0.01) so that its Uij components approximate to isotropic. The enhanced rigid-bond restraint was applied to the disordered fluorine atoms and anthracene.[6] The highest peaks in the difference map were located around the disordered anthracene indicating some more possible disorder. CCDC Number: 913425.

3) Ex^{2}Box⊂Pyrene•$4PF_6$(Pyrene)

a) Method. Solid pyrene (1.5 mg, 7.2 μmol) was added to a solution of **Ex^{2}Box**•$4PF_6$ (3.4 mg, 2.4 μmol) in MeCN (0.8 mL) and, after it dissolved, the mixture was passed through a 0.45-μm

filter equally into three 1-mL tubes. The tubes were placed together in one 20-mL vial containing *i*Pr_2O (~3 mL) and the vial was capped. Slow vapor diffusion of *i*Pr_2O into the 3:1 solution of pyrene and **Ex^{2}Box**•4PF_6 in MeCN over the period of 7 d yielded yellow single crystals of **Ex^{2}Box**⊂pyrene•4PF_6(pyrene). Data were collected at 100 K on a Bruker Kappa APEX2 CCD Diffractometer equipped with a CuK_α microsource with Quazar optics. The solid-state superstructure of **Ex^{2}Box^{4+}**⊂pyrene•(pyrene) is shown in Figure S3.

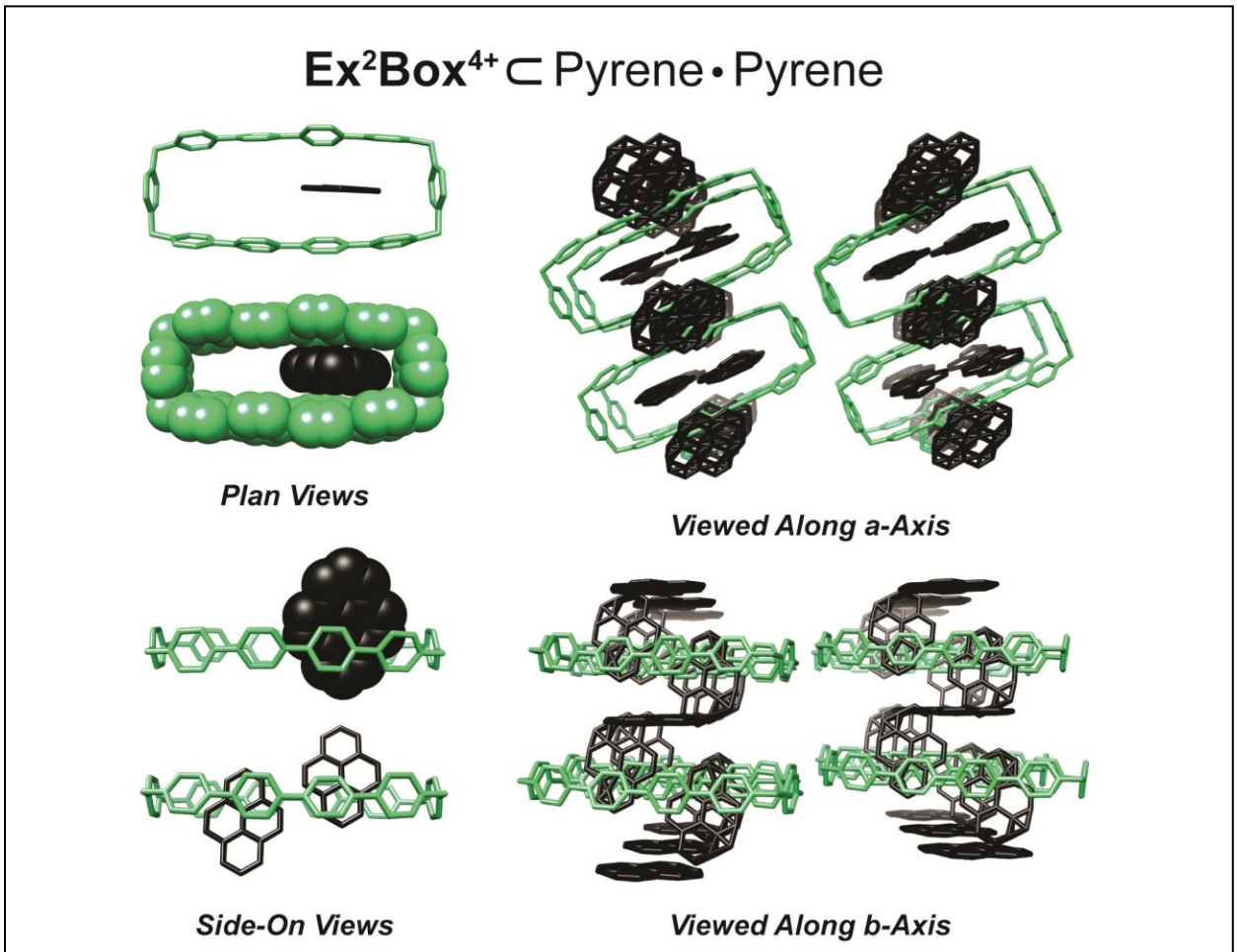


Figure S3. Different crystallographic views of **Ex^{2}Box^{4+}**⊂pyrene•(pyrene). Each **Ex^{2}Box^{4+}** cyclophane is occupied with one molecule of pyrene. Pyrene molecules are disordered and each molecule of pyrene can be positioned in two different ways within **Ex^{2}Box^{4+}** cyclophane (bottom-left). Counterions and solvent molecules are omitted for the sake of clarity.

b) Crystal Parameters. $[C_{60}H_{48}N_4 \subset C_{16}H_{10} \bullet (PF_6)_4] \bullet (C_{16}H_{10}) \bullet (MeCN)_4$. Yellow block (0.22 × 0.13 × 0.09 mm). Triclinic, $P\bar{1}$, a = 10.280(3), b = 11.369(3), c = 21.540(6) Å, α = 78.670(13), β = 84.909(13), γ = 64.499(13)º, V = 2227.88(11) Å^3, Z = 1, T = 100.03 K, ρ_{calc} = 1.471 g cm^{-3}, μ = 0.190 mm^{-1}. Of a total of 61143 reflections that were collected, 12838 were unique. Final R_1 =

0.0910 and wR_2 = 0.2082. Distance restraints were refined for the disordered pyrene molecules. The enhanced rigid-bond restraint was applied[6] globally. CCDC Number: 913426.

4) $Ex^2Box\subset(Tetraphene)_{0.5}\bullet 4PF_6(Tetraphene)_{0.5}$

a) Method. Solid tetraphene (1.0 mg, 4.4 μmol) was added to a solution of **$Ex^2Box\bullet 4PF_6$** (1.0 mg, 0.71 μmol) in MeCN (0.8 mL) and, after it dissolved, the mixture was passed through a 0.45-μm filter equally into three 1-mL tubes. The tubes were placed together in one 20-mL vial containing *i*Pr_2O (~3 mL) and the vial was capped. Slow vapor diffusion of *i*Pr_2O into the 6.2:1 solution of tetraphene and **$Ex^2Box\bullet 4PF_6$** in MeCN over the course of 2 d yielded colorless single crystals of **$Ex^2Box\subset(tetraphene)_{0.5}\bullet 4PF_6(tetraphene)_{0.5}$.** Data were collected at 100 K on a Bruker Kappa APEX2 CCD Diffractometer equipped with a CuK_α microsource with Quazar optics. The solid-state superstructure of **$Ex^2Box^{4+}\subset(tetraphene)_{0.5}\bullet(tetraphene)_{0.5}$** is shown in Figure S4.

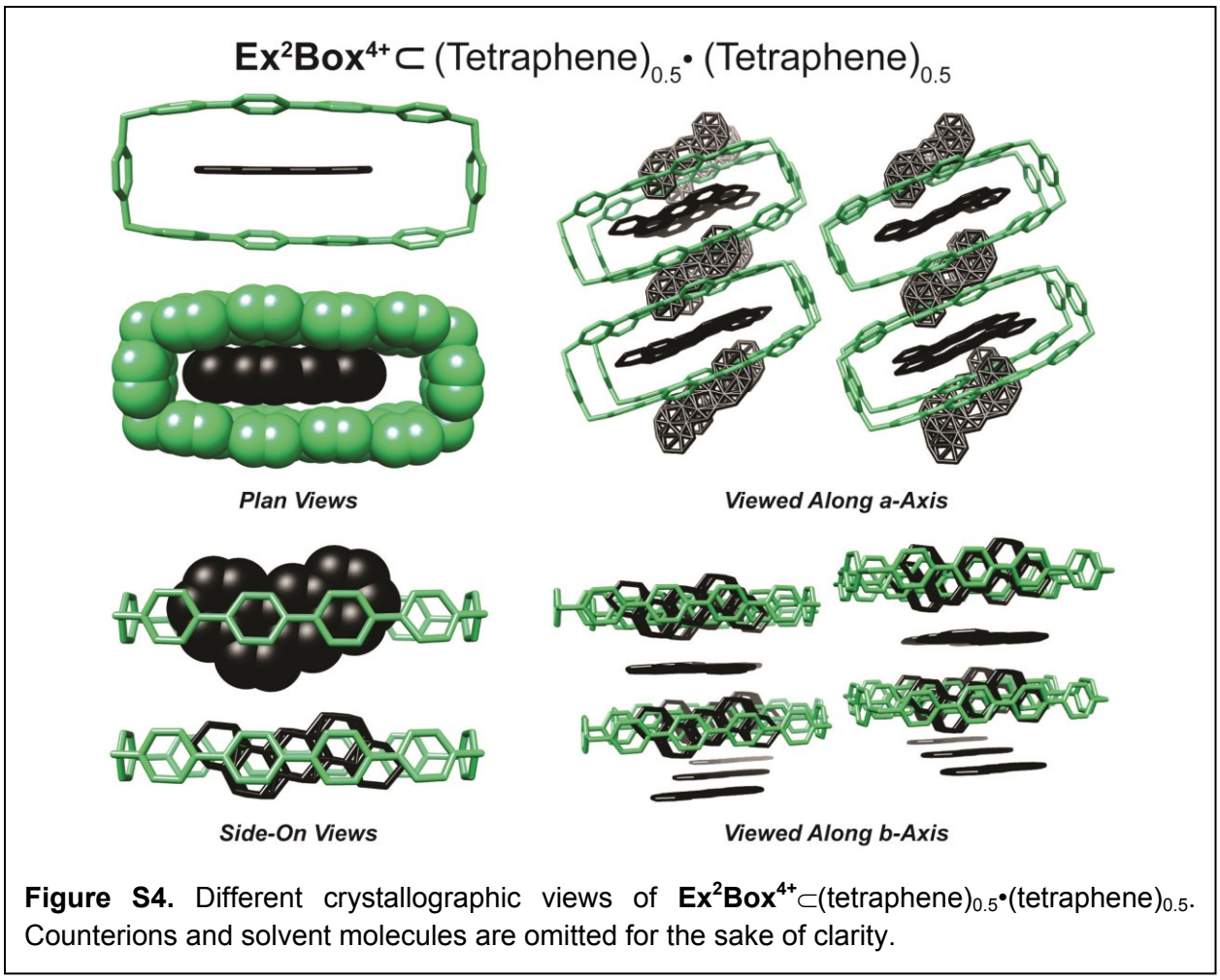


Figure S4. Different crystallographic views of **$Ex^2Box^{4+}\subset(tetraphene)_{0.5}\bullet(tetraphene)_{0.5}$**. Counterions and solvent molecules are omitted for the sake of clarity.

b) Crystal Parameters. $[C_{60}H_{48}N_4 \subset (C_{18}H_{12})_{0.5} \bullet (PF_6)_4] \bullet (C_{18}H_{12})_{0.5} \bullet (MeCN)_3$. Colorless block (0.11 × 0.08 × 0.04 mm). Triclinic, $P\bar{1}$, a = 10.415(7), b = 11.339(9), c = 21.467(14) Å, α = 79.584(18), β = 85.427(13), γ = 65.790(2)°, V = 2274.0(3) Å^3, Z = 1, T = 99.98 K, ρ_{calc} = 1.283 g cm^{-3}, μ = 1.595 mm^{-1}. Of a total of 14610 reflections that were collected, 7508 were unique. Final R_1 = 0.1060 and wR_2 = 0.3191. Distant restraints were imposed on bonds, rigid-bond restraints (esd 0.01) were imposed on the displacement parameters as well as restraints on similar amplitudes (esd 0.05) separated by less than 1.7 Å on all disordered atoms. The disordered tetraphene molecules were restrained (esd 0.01) so that their Uij components approximate to isotropic. CCDC Number: 936766.

5) Ex^{2}Box⊂Chrysene•4PF$_6$(Chrysene)

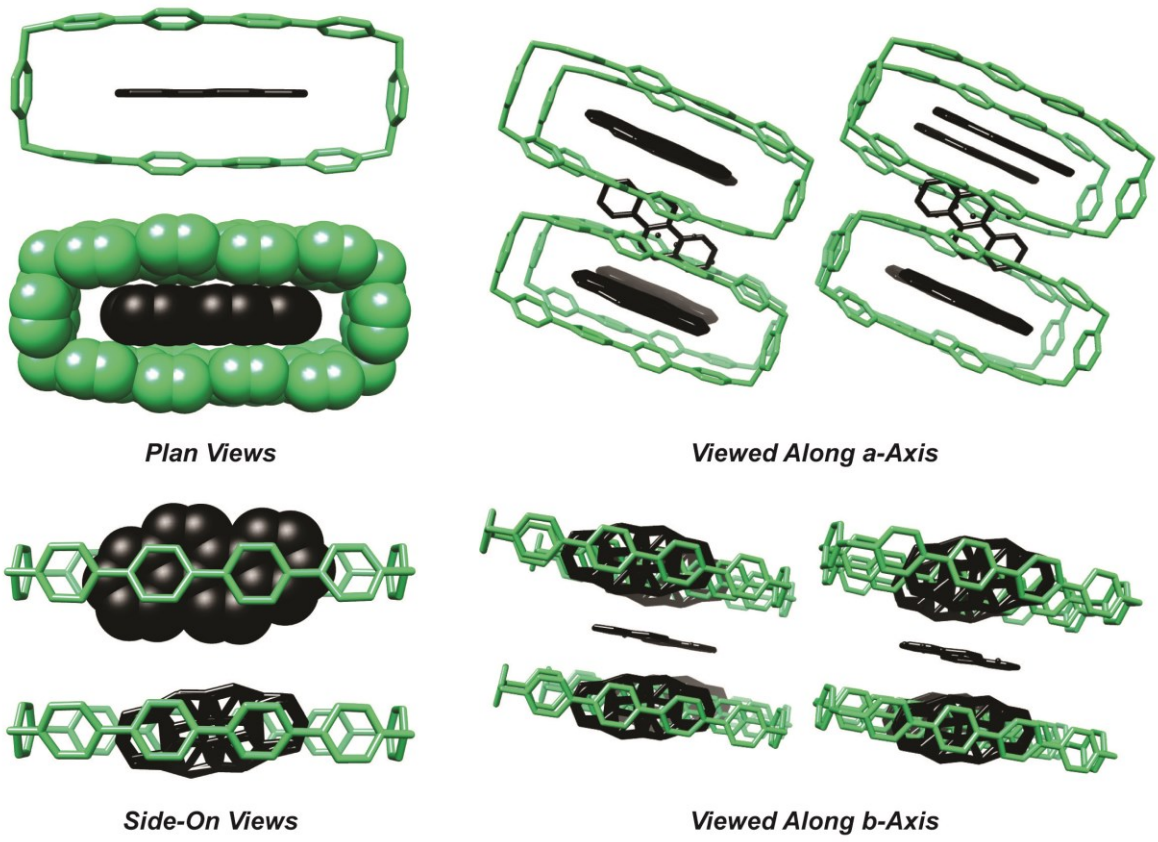


Figure S5. Different crystallographic views of **Ex^{2}Box^{4+}**⊂chrysene•(chrysene). Counterions and solvent molecules are omitted for the sake of clarity.

a) Method. Solid chrysene (0.7 mg, 3 μmol) was added to a solution of **Ex^{2}Box**•4PF_6 (2.0 mg, 1.4 μmol) in MeCN (0.8 mL) and, after it dissolved, the mixture was passed through a 0.45-μm filter equally into three 1-mL tubes. The tubes were placed together in one 20-mL vial containing *i*Pr_2O (~3 mL) and the vial was capped. Slow vapor diffusion of *i*Pr_2O into the 2.1:1 solution of chrysene and **Ex^{2}Box**•4PF_6 in MeCN over the course of 4 d yielded colorless single crystals of **Ex^{2}Box**⊂chrysene•4PF_6(chrysene). Data were collected at 100 K on a Bruker Kappa APEX2 CCD Diffractometer equipped with a CuK_α microsource with Quazar optics. The solid-state superstructure of **Ex^{2}Box^{4+}**⊂chrysene•(chrysene) is shown in Figure S5.

b) Crystal Parameters. $[C_{60}H_{48}N_4 \subset C_{18}H_{12} \bullet (PF_6)_4] \bullet (C_{18}H_{12}) \bullet (MeCN)_4$. Colorless block (0.19 × 0.10 × 0.01 mm). Triclinic, $P\bar{1}$, a = 10.480(4), b = 11.349(5), c = 21.442(9) Å, α = 80.25(3), β = 86.77(3), γ = 64.519(2)°, V = 2268.6(17) Å^3, Z = 1, T = 100.12 K, ρ_{calc} = 1.483 g cm^{-3}, μ = 1.687 mm^{-1}. Of a total of 14871 reflections that were collected, 7507 were unique. Final R_1 = 0.0447 and wR_2 = 0.1137. Rigid bond restraints (esd 0.01) were imposed on the displacement parameters as well as restraints on similar amplitudes (esd 0.05) separated by less than 1.7 Å on the disordered carbon atoms of chrysene. Similar distances (SADI) and a flat command were also refined for these carbon atoms. CCDC Number: 936767.

6) Ex^{2}Box⊂ Tetracene•4PF_6(Tetracene)

a) Method. A mixture of tetracene (0.30 mg, 1.3 μmol), **Ex^{2}Box**•4PF_6 (1.7 mg, 1.2 μmol), MeCN (0.8 mL), and PhMe (0.8 mL) was heated at 80 ºC for 30 min before an additional portion of MeCN (0.8 mL) was added. The resulting solution was then allowed to cool slowly to room temperature and was passed through a 0.45-μm filter equally into six 1-mL tubes. The tubes were placed in two 20-mL vials (three in each) containing *i*Pr_2O (2 mL) and the vials were capped. Slow vapor diffusion of *i*Pr_2O into the 1.1:1 solution of tetracene and **Ex^{2}Box**•4PF_6 in MeCN/PhMe over the period of 1 d yielded orange single crystals of **Ex^{2}Box**⊂tetracene•4PF_6(tetracene). Data were collected at 100 K on a Bruker Kappa APEX2 CCD Diffractometer equipped with a CuK_α microsource with Quazar optics. The solid-state superstructure of **Ex^{2}Box^{4+}**⊂tetracene•(tetracene) is shown in Figure S6.

b) Crystal Parameters. $[C_{60}H_{48}N_4 \subset (C_{18}H_{12}) \bullet (PF_6)_4] \bullet (C_{18}H_{12}) \bullet (MeCN)_4$. Orange block (0.23 × 0.10 × 0.02 mm). Triclinic, $P\bar{1}$, a = 10.480(3), b = 11.384(3), c = 21.556(6) Å, α = 80.426(2), β = 86.407(17), γ = 63.302(16)º, V = 2265.29(11) Å^3, Z = 1, T = 99.95 K, ρ_{calc} = 1.448 g cm^{-3}, μ =

1.689 mm^{-1}. Of a total of 14958 reflections that were collected, 7309 were unique. Final R_1 = 0.0546 and wR_2 = 0.1575. No special refinement was necessary. CCDC Number: 913427.

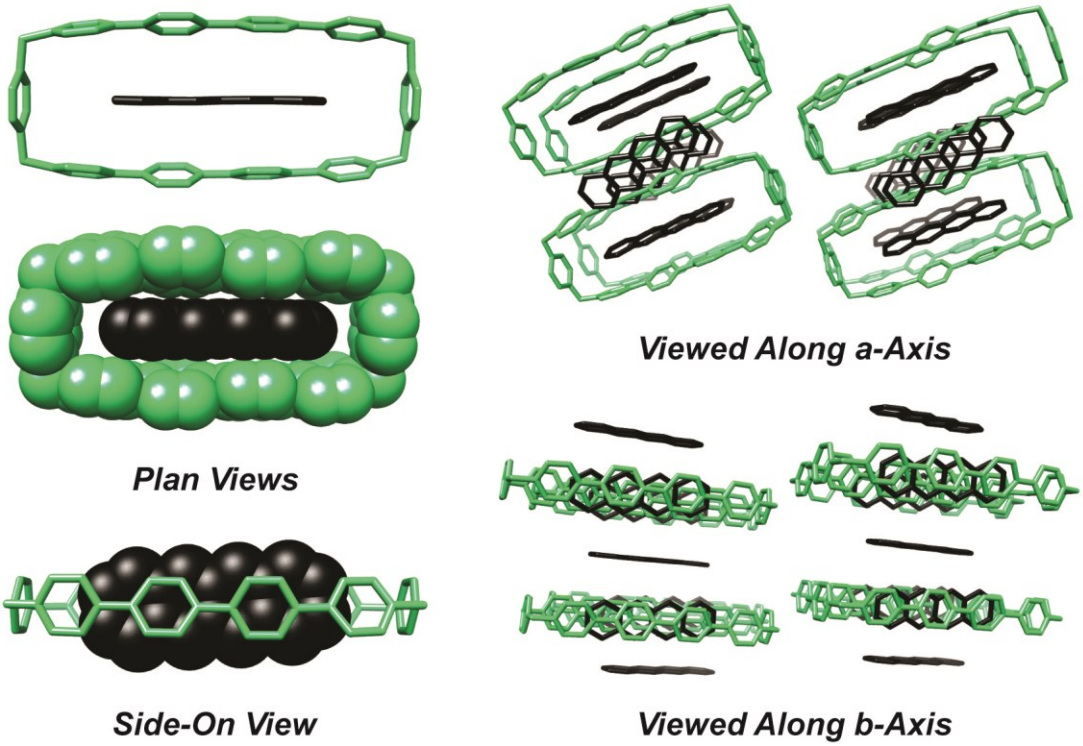


Figure S6. Different crystallographic views of **Ex²Box⁴⁺**⊂tetracene•(tetracene)**.** Counterions and solvent molecules are omitted for the sake of clarity.

7) Ex²Box⊂(2,6-Dinitrotoluene)•4PF₆

a) Method. Solid 2,6-dinitrotoluene (4.0 mg, 22 μmol) was added to a solution of **Ex²Box**•4PF_6 (3.3 mg, 2.3 μmol) in MeCN (0.8 mL) and, after it dissolved, the mixture was passed through a 0.45-μm filter equally into three 1-mL tubes. The tubes were placed together in one 20-mL vial containing *i*Pr_2O (~3 mL) and the vial was capped. Slow vapor diffusion of *i*Pr_2O into the 10:1 solution of 2,6-dinitrotoluene and **Ex²Box**•4PF_6 in MeCN over the period of 4 d yielded colorless single crystals of **Ex²Box**⊂(2,6-dinitrotoluene)•4PF_6**.** Data were collected at 100 K on a Bruker Kappa APEX2 CCD Diffractometer equipped with a CuK_α microsource with MX optics. The solid-state superstructure of **Ex²Box⁴⁺**⊂(2,6-dinitrotoluene) is shown in Figure S7.

b) Crystal Parameters. $[C_{60}H_{48}N_4 \subset C_7H_6N_2O_4 \bullet (PF_6)_4]$. Colorless block (0.17 × 0.08 × 0.03 mm). Orthorhombic, *Cmca*, a = 14.443(6), b = 38.482(14), c = 12.120(4) Å, α = 90.000, β = 90.000, γ = 90.000º, V = 6735.9(4) Å^3, Z = 4, T = 99.99 K, ρ_{calc} = 1.565 g cm^{-3}, μ = 2.125 mm^{-1}. Of a total of 13160 reflections that were collected, 2799 were unique. Final R_1 = 0.0791 and wR_2 = 0.2195. 2,6-Dinitrotoluene (DNT) is disordered over several symmetry elements and refined without special position constraints (PART –1). The atoms of the toluene benzenoid ring were refined with a perfect hexagon restraint (AFIX 66), and the C_{Ar}–CH_3, C–N, and N–O distances were refined with appropriate distance restraints as taken from a search of similar compounds in the Cambridge Structural Database. A group displacement parameter was used for the anisotropic refinement of the disordered DNT molecule. CCDC Number: 913429.

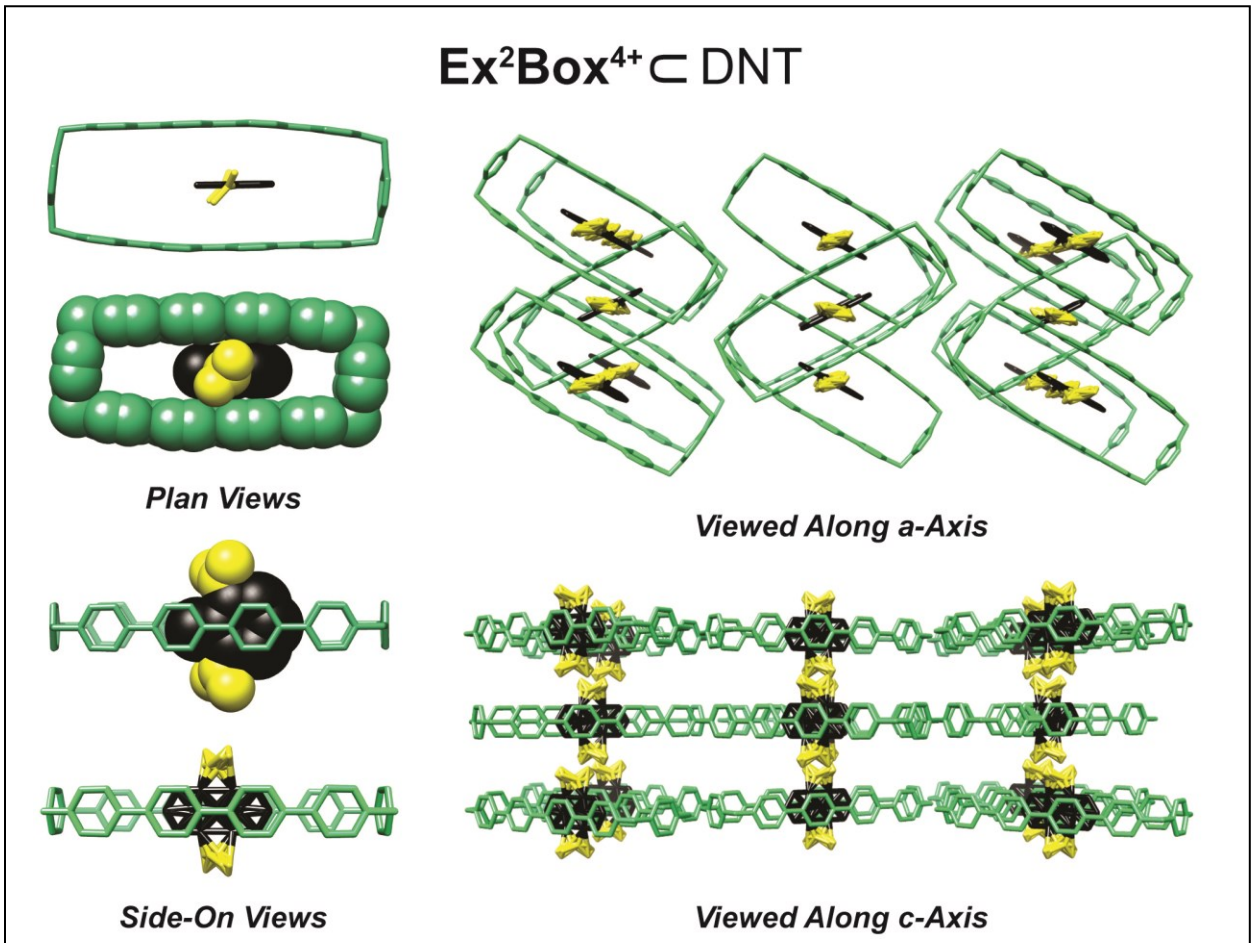


Figure S7. Different crystallographic views of **Ex^{2}Box^{4+}**⊂(2,6-dinitrotoluene)**.** Each **Ex^{2}Box^{4+}** cyclophane is occupied with one molecule of 2,6-dinitrotoluene. 2,6-Dinitrotoluene molecules are disordered and can be positioned in several different ways within **Ex^{2}Box^{4+}** cyclophane (bottom-left). Counterions are omitted for the sake of clarity. DNT = 2,6-dinitrotoluene.

8) Ex²Box⊂(1,5-Dinitronaphthalene)•4PF₆

a) Method. Solid 1,5-dinitronaphthalene (6.2 mg, 28 μmol) was added to a solution of **Ex²Box**•4PF_6 (2.0 mg, 1.4 μmol) in MeCN (0.8 mL) and, after it dissolved, the mixture was passed through a 0.45-μm filter equally into three 1-mL tubes. The tubes were placed together in one 20-mL vial containing *i*Pr_2O (~3 mL) and the vial was capped. Slow vapor diffusion of *i*Pr_2O into the 20:1 solution of 1,5-dinitronaphthalene and **Ex²Box**•4PF_6 in MeCN over the course of 7 d yielded yellow single crystals of **Ex²Box**⊂(1,5-dinitronaphthalene)•4PF_6**.** Data were collected at 100 K on a Bruker Kappa APEX2 CCD Diffractometer equipped with a CuK_α microsource with Quazar optics. The solid-state superstructure of **Ex²Box⁴⁺**⊂(1,5-dinitronaphthalene) is shown in Figure S8.

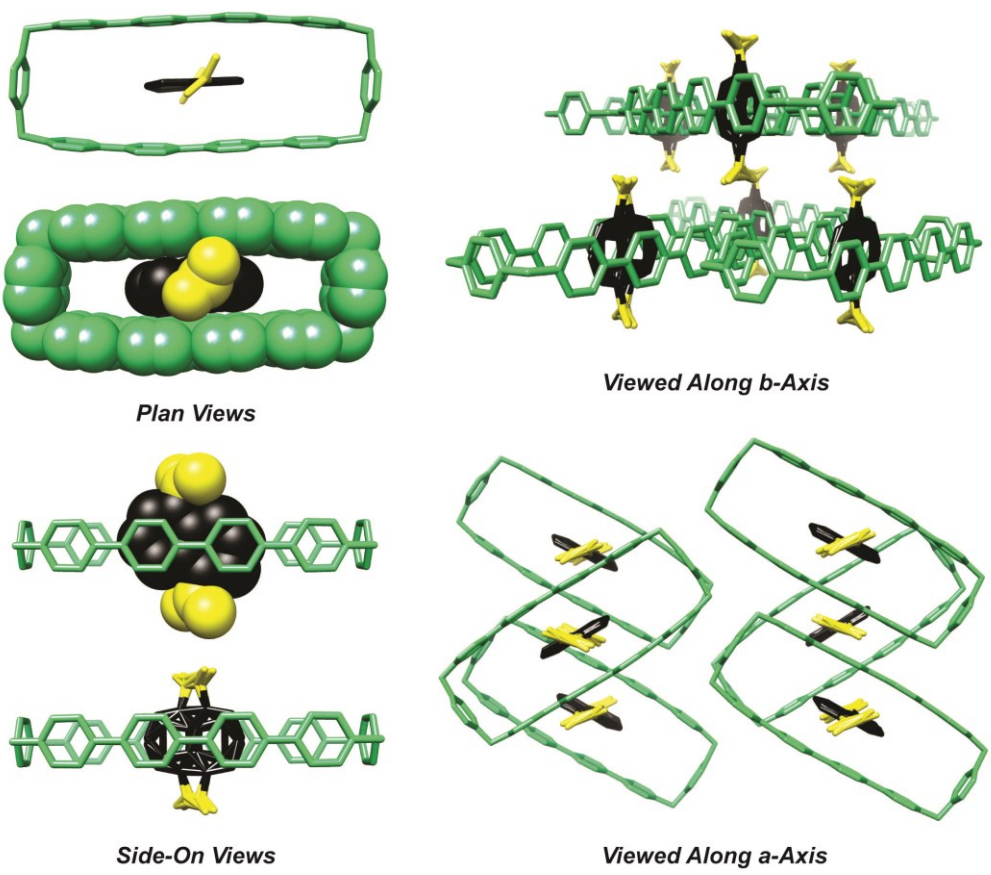


Figure S8. Different crystallographic views of **Ex²Box⁴⁺**⊂(1,5-dinitronaphthalene)**.** 1,5-Dinitronaphthalene molecules are disordered and can be positioned in several different ways within **Ex²Box⁴⁺** cyclophane (bottom-left). Counterions are omitted for the sake of clarity. DNN = 1,5-dinitronaphthalene.

b) Crystal Parameters. [$C_{60}H_{48}N_4 \subset C_{10}H_6N_2O_4 \bullet (PF_6)_4$]. Yellow block (0.19 × 0.16 × 0.01 mm). Orthorhombic, *Cmca*, a = 14.913(6), b = 38.067(17), c = 12.106(5) Å, α = 90.000, β = 90.000, γ = 90.000°, V = 6872.8(5) Å^3, Z = 4, T = 100.01 K, ρ_{calc} = 1.569 g cm^{-3}, μ = 2.098 mm^{-1}. Of a total of 13018 reflections that were collected, 3017 were unique. Final R_1 = 0.0422 and wR_2 = 0.0994. Rigid-bond restraints were imposed on the displacement parameters as well as restraints on similar amplitudes separated by less than 1.7 Å on the disordered 1,5-dinitronaphthalene (DNN). The oxygen atoms were restrained so that their Uij components approximate to isotropic. Distance restraints were also imposed on the disordered DNN molecule. CCDC Number: 936768.

9) Ex^{2}Box⊂(9,10-Anthraquinone)$_{0.5}$•4PF$_6$

a) Method. Solid 9,10-anthraquinone (6.3 mg, 30 μmol) was added to a solution of **Ex^{2}Box**•4PF$_6$ (2.2 mg, 1.6 μmol) in MeCN (0.8 mL) and, after it dissolved, the mixture was passed through a 0.45-μm filter equally into three 1-mL tubes. The tubes were placed together in one 20-mL vial containing *i*Pr$_2$O (~3 mL) and the vial was capped. Slow vapor diffusion of *i*Pr$_2$O into the 19:1 solution of 9,10-anthraquinone and **Ex^{2}Box**•4PF$_6$ in MeCN over the course of 7 d yielded yellow single crystals of **Ex^{2}Box**⊂(9,10-anthraquinone)$_{0.5}$•4PF$_6$**.** Note the structural formula in the *Crystal Parameters* section below reflects an occupancy of only half of the **Ex^{2}Box**•4PF$_6$ cyclophanes with 9,10-anthraquinone molecules. Data were collected at 100 K on a Bruker Kappa APEX2 CCD Diffractometer using a CuK$_\alpha$ microsource with Quazar optics. The solid-state superstructure of **Ex^{2}Box^{4+}**⊂(9,10-anthraquinone)$_{0.5}$ is shown in Figure S9.

b) Crystal Parameters. [$C_{60}H_{48}N_4 \subset (C_{14}H_{10}O_2)_{0.5} \bullet (PF_6)_4$]•MeCN. Yellow block (0.05 × 0.05 × 0.03 mm). Monoclinic, $P2_1/c$, a = 20.082(37), b = 12.103(4), c = 14.458(6) Å, α = 90.000, β = 106.223(3), γ = 90.000º, V = 3374.2(2) Å^3, Z = 2, T = 100.01 K, ρ_{calc} = 1.528 g cm^{-3}, μ = 2.068 mm^{-1}. Of a total of 4115 reflections that were collected, 4115 were unique. Final R_1 = 0.0636 and wR_2 = 0.1751. The crystal under investigation was found to be non-merohedrally twinned. The orientation matrices for the two components were identified using the program Cell Now,[4] and the data were processed using both orientation matrices with SAINT. The exact twin matrix identified by the integration program was found to be –1.00119 –0.00053 –0.00309 / 0.00035 –1.00000 –0.00004 / 0.77107 0.00010 1.00119. The second domain is rotated from the first domain by 179.9° about the reciprocal lattice *a*-axis (reduced cell). The absorption correction

was carried out using TWINABS V2008/4[5] to create an hklf5 file that was used in all refinements; the structure was solved using direct methods with only the non-overlapping reflections of component 1. The twin fraction refined to a value of 0.351(2). CCDC Number: 913430.

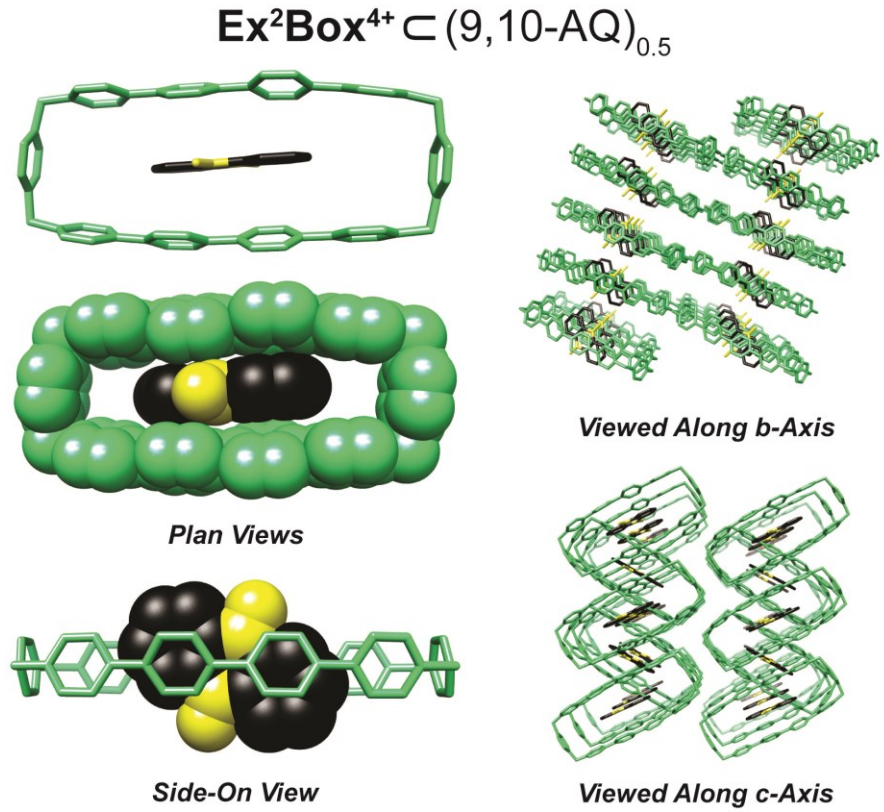


Figure S9. Different crystallographic views of **Ex^{2}Box^{4+}**⊂(9,10-anthraquinone)$_{0.5}$. Half of the **Ex^{2}Box^{4+}** cyclophanes are occupied with one 9,10-anthraquinone molecule and half of the **Ex^{2}Box^{4+}** cyclophanes are occupied with one MeCN molecule. Counterions and solvent molecules are omitted for the sake of clarity. 9,10-AQ = 9,10-anthraquinone.

10) Ex^{2}Box⊂(1,4-Anthraquinone)•4PF$_6$

a) Method. A solution of 1,4-anthraquinone (5.9 mg, 28 μmol) in $CHCl_3$ (0.2 mL) was added to a solution of **Ex^{2}Box**•4PF_6 (2.0 mg, 1.4 μmol) in MeCN (0.8 mL) and the mixture was passed through a 0.45-μm filter equally into three 1-mL tubes. The tubes were placed together in one 20-mL vial containing *i*Pr_2O (~3 mL) and the vial was capped. Slow vapor diffusion of *i*Pr_2O into the 20:1 solution of 1,4-anthraquinone and **Ex^{2}Box**•4PF_6 in MeCN/$CHCl_3$ over the course of 7 d yielded yellow single crystals of **Ex^{2}Box**⊂(1,4-anthraquinone)•4PF_6**.** Data were collected at

100 K on a Bruker Kappa APEX2 CCD Diffractometer equipped with a CuK_α microsource with Quazar optics. The solid-state superstructure of **Ex^{2}Box^{4+}**⊂(1,4-anthraquinone) is shown in Figure S10.

b) Crystal Parameters. $[C_{60}H_{48}N_4 \subset C_{14}H_8O_2 \bullet (PF_6)_4] \bullet (CHCl_3)_2$. Yellow block (0.45 × 0.14 × 0.12 mm). Monoclinic, $P2_1/c$, a = 9.790(4), b = 14.131(6), c = 27.617(12) Å, α = 90.000, β = 95.911(2), γ = 90.000º, V = 3800.4(3) Å^3, Z = 2, T = 100.0 K, ρ_{calc} = 1.618 g cm^{-3}, μ = 0.421 mm^{-1}. Of a total of 57735 reflections that were collected, 11430 were unique. Final R_1 = 0.0722 and wR_2 = 0.2057. The enhanced rigid-bond restraint was applied[6] globally. CCDC Number: 936769.

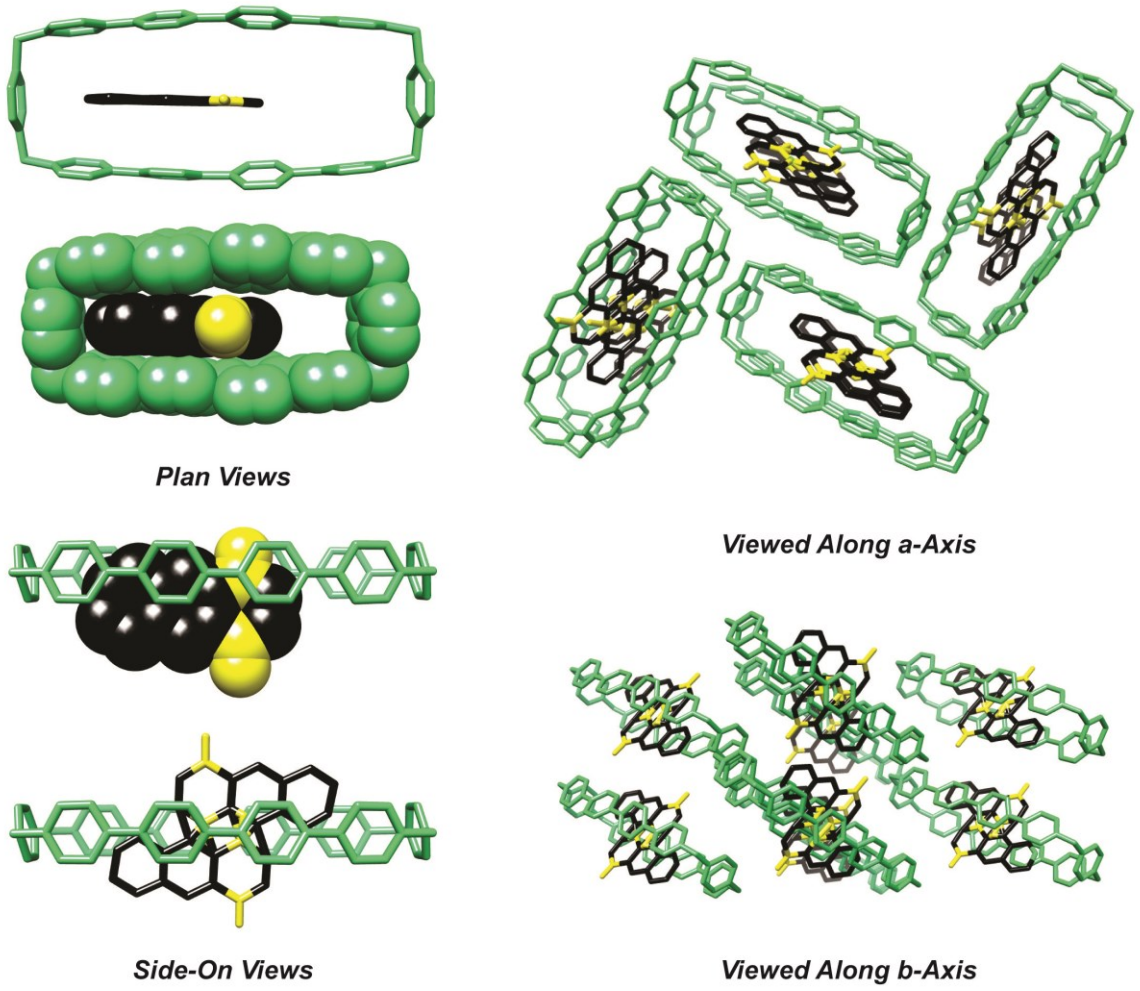


Figure S10. Different crystallographic views of **Ex^{2}Box^{4+}**⊂(1,4-anthraquinone)**.** Counterions and solvent molecules are omitted for the sake of clarity. 1,4-AQ = 1,4-anthraquinone.

11) Ex^2Box⊂[1,4-Bis(3-methoxyphenyl)-1H-1,2,3-triazole]•4PF_6[1,4-Bis(3-methoxyphenyl)-1H-1,2,3-triazole]

a) Method. Solid 1,4-Bis(3-methoxyphenyl)-1*H*-1,2,3-triazole (BMPT) (2.0 mg, 6.4 μmol) was added to a solution of **Ex^2Box**•4PF_6 (2.0 mg, 1.4 μmol) in MeCN (0.8 mL) and, after it dissolved, the mixture was passed through a 0.45-μm filter equally into three 1-mL tubes. The tubes were placed together in one 20-mL vial containing *i*Pr_2O (~3 mL) and the vial was capped. Slow vapor diffusion of *i*Pr_2O into the 4.6:1 solution of BMPT and **Ex^2Box**•4PF_6 in MeCN over the course of 6 d yielded yellow single crystals of **Ex^2Box**⊂BMPT•4PF_6(BMPT). Data were collected at 100 K on a Bruker Kappa APEX2 CCD Diffractometer equipped with a CuK_α microsource with Quazar optics. The solid-state superstructure of **Ex^2Box^{4+}**⊂BMPT•(BMPT) is shown in Figure S11.

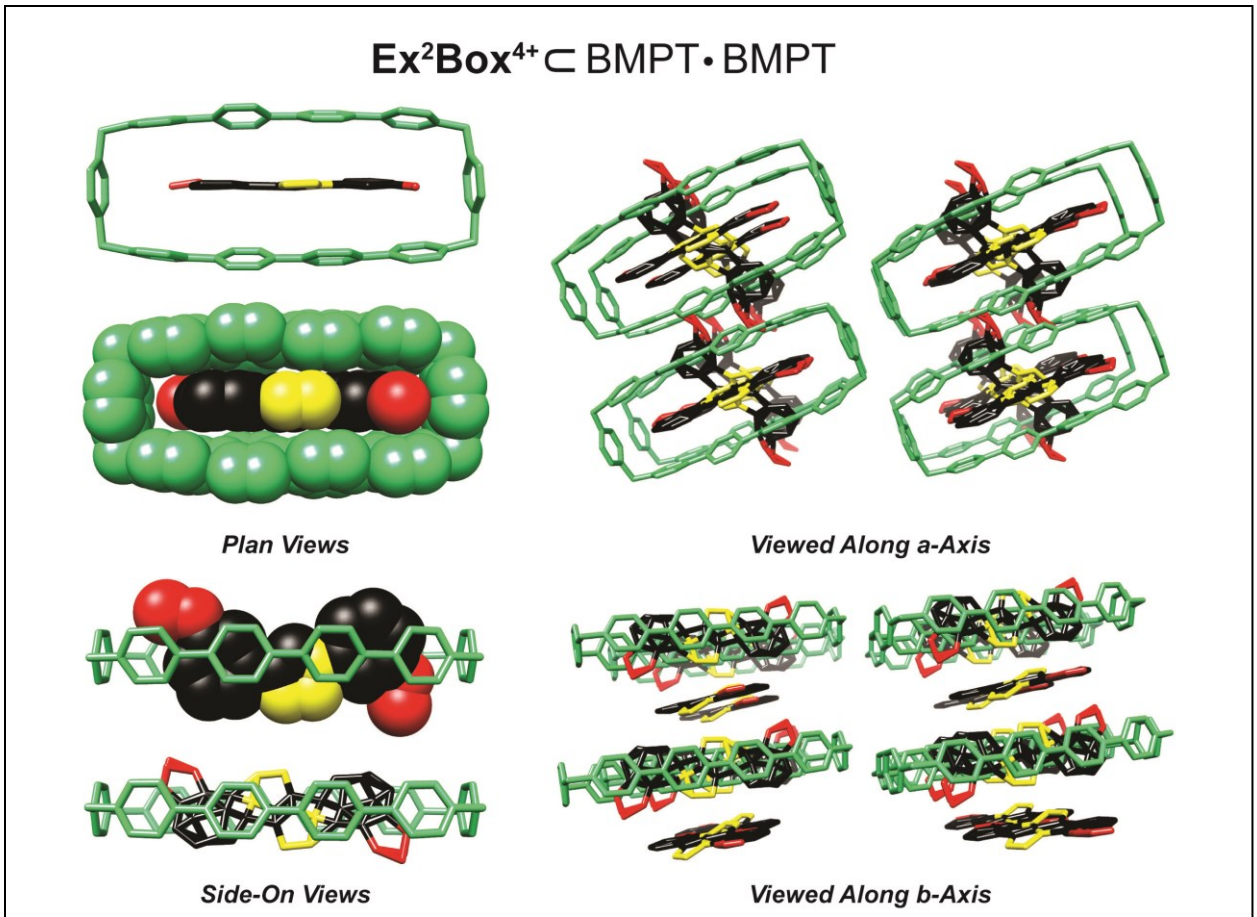


Figure S11. Different crystallographic views of **Ex^2Box^{4+}**⊂BMPT. The BMPT molecules are disordered and can be positioned in several different ways within **Ex^2Box^{4+}** cyclophane (bottom-left). Counterions and solvent molecules are omitted for the sake of clarity.

b) Crystal Parameters. $[C_{60}H_{48}N_4 \subset C_{16}H_{15}N_3O_2 \bullet (PF_6)_4] \bullet (C_{16}H_{15}N_3O_2) \bullet (MeCN)_{2.5}$. Colorless block (0.11 × 0.08 × 0.04 mm). Triclinic, $P\bar{1}$, a = 10.4059(3), b = 11.3697(3), c = 21.2021(5) Å, α = 81.1853(12), β = 86.2716(13), γ = 64.9951(11)°, V = 2246.50(10) Å^3, Z = 1, T = 100.03 K, ρ_{calc} = 1.530 g cm^{-3}, μ = 0.197 mm^{-1}. Of a total of 90082 reflections that were collected, 13104 were unique. Final R_1 = 0.1051 and wR_2 = 0.2775. Similar distance restraints were applied to the disordered atoms. The enhanced rigid-bond restraint was applied[6] globally. CCDC Number: 936770.

12) Ex^{2}Box⊂(1,2,4-Trichlorobenzene)$_2$•4PF$_6$(Tetracene)

a) Method. A mixture of tetracene (0.30 mg, 1.3 μmol), **Ex^{2}Box**•4PF$_6$ (1.7 mg, 1.2 μmol), MeCN (0.8 mL), and 1,2,4-trichlorobenzene (0.8 mL) was heated at 90 ºC for 30 min before an additional portion of MeCN (0.8 mL) was added. The resulting solution was then allowed to cool slowly to room temperature and was passed through a 0.45-μm filter equally into six 1-mL tubes. The tubes were placed in two 20-mL vials (three in each) containing *i*Pr$_2$O (~1.5 mL) and the vials were capped. Slow vapor diffusion of *i*Pr$_2$O into the 1.1:1 solution of tetracene and **Ex^{2}Box**•4PF$_6$ in MeCN/1,2,4-trichlorobenzene over the period of 3 d yielded yellow single crystals of **Ex^{2}Box**⊂(1,2,4-trichlorobenzene)$_2$•4PF$_6$(tetracene). Data were collected at 100 K on a Bruker Kappa APEX2 CCD Diffractometer equipped with a CuK$_\alpha$ microsource with Quazar optics. The solid-state superstructure of **Ex^{2}Box^{4+}**⊂(1,2,4-trichlorobenzene)$_2$•(tetracene) is shown in Figure S12.

b) Crystal Parameters. $[C_{60}H_{48}N_4 \subset (C_6H_3Cl_3)_2 \bullet (PF_6)_4] \bullet (C_{18}H_{12}) \bullet (MeCN)_4$. Yellow block (0.21 × 0.12 × 0.04 mm). Triclinic, $P\bar{1}$, a = 10.779(3), b = 11.107(3), c = 21.133(5) Å, α = 81.978(10), β = 88.551(10), γ = 67.138(10)º, V = 2307.3(10) Å^3, Z = 1, T = 99.99 K, ρ_{calc} = 1.555 g cm^{-3}, μ = 3.257 mm^{-1}. Of a total of 22031 reflections that were collected, 7769 were unique. Final R_1 = 0.0435 and wR_2 = 0.1208. No restraints or constraints were used in this refinement. CCDC Number: 913423.

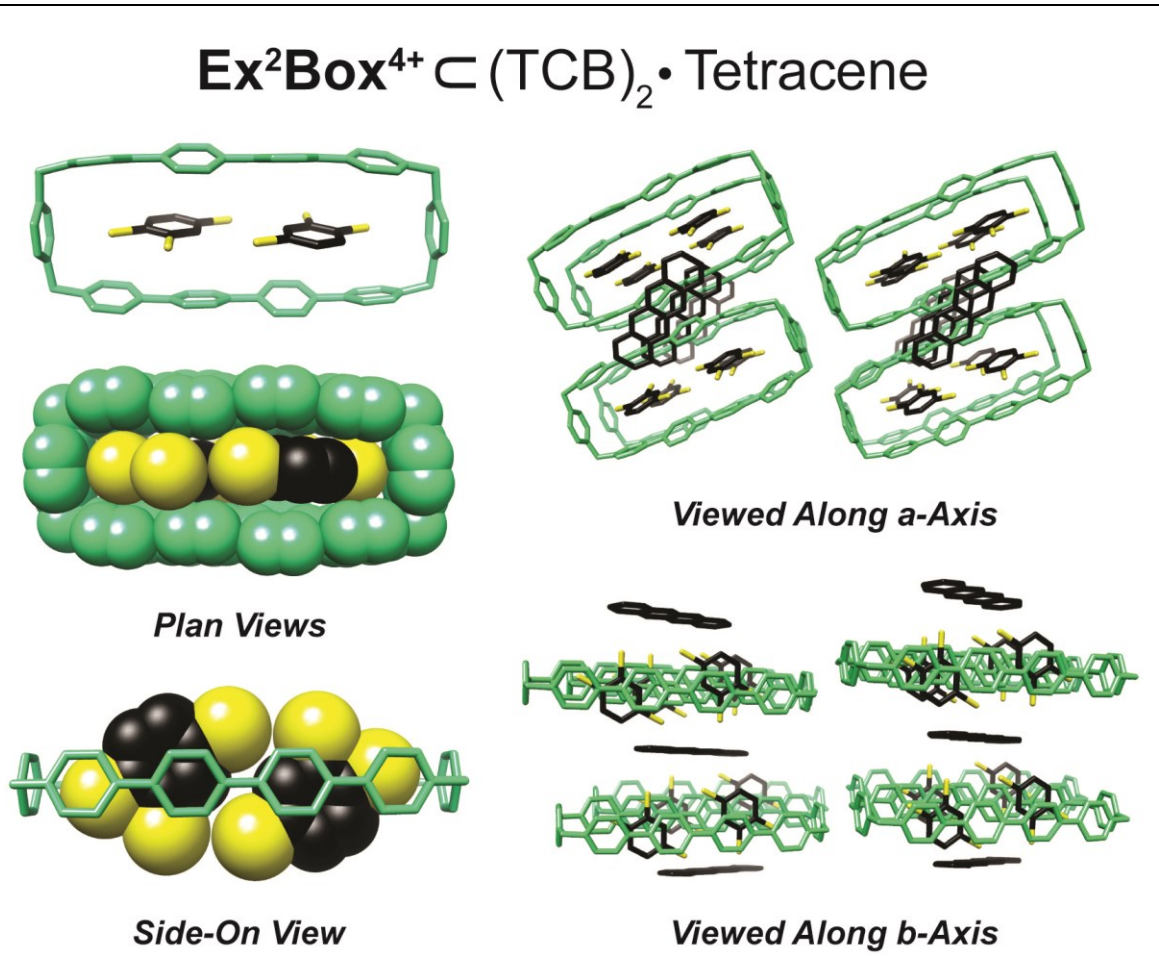


Figure S12. Different crystallographic views of **Ex^{2}Box^{4+}**⊂(1,2,4-trichlorobenzene)$_2$• (tetracene)**.** Counterions and solvent molecules are omitted for the sake of clarity. TCB = 1,2,4-trichlorobenzene.

13) Ex^{2}Box⊂(1,5-Dinaphtho[38]crown-10)•4PF$_6$

a) Method. Solid 1,5-dinaphtho[38]crown-10 (30 mg, 48 μmol) was added to a solution of **Ex^{2}Box**•4PF$_6$ (3.4 mg, 2.4 μmol) in MeCN (0.8 mL) and, after it dissolved, the mixture was passed through a 0.45-μm filter equally into three 1-mL tubes. The tubes were placed together in one 20-mL vial containing *i*Pr$_2$O (~3 mL) and the vial was capped. Slow vapor diffusion of *i*Pr$_2$O into the 20:1 solution of 1,5-dinaphtho[38]crown-10 and **Ex^{2}Box**•4PF$_6$ in MeCN over the course of 7 d yielded orange single crystals of **Ex^{2}Box**⊂(1,5-dinaphtho[38]crown-10)•4PF$_6$**.** Data were collected at 100 K on a Bruker Kappa APEX2 CCD Diffractometer equipped with a CuK$_\alpha$ microsource with Quazar optics. The solid-state superstructure of **Ex^{2}Box^{4+}**⊂(1,5-dinaphtho[38]crown-10) is shown in Figure S13.

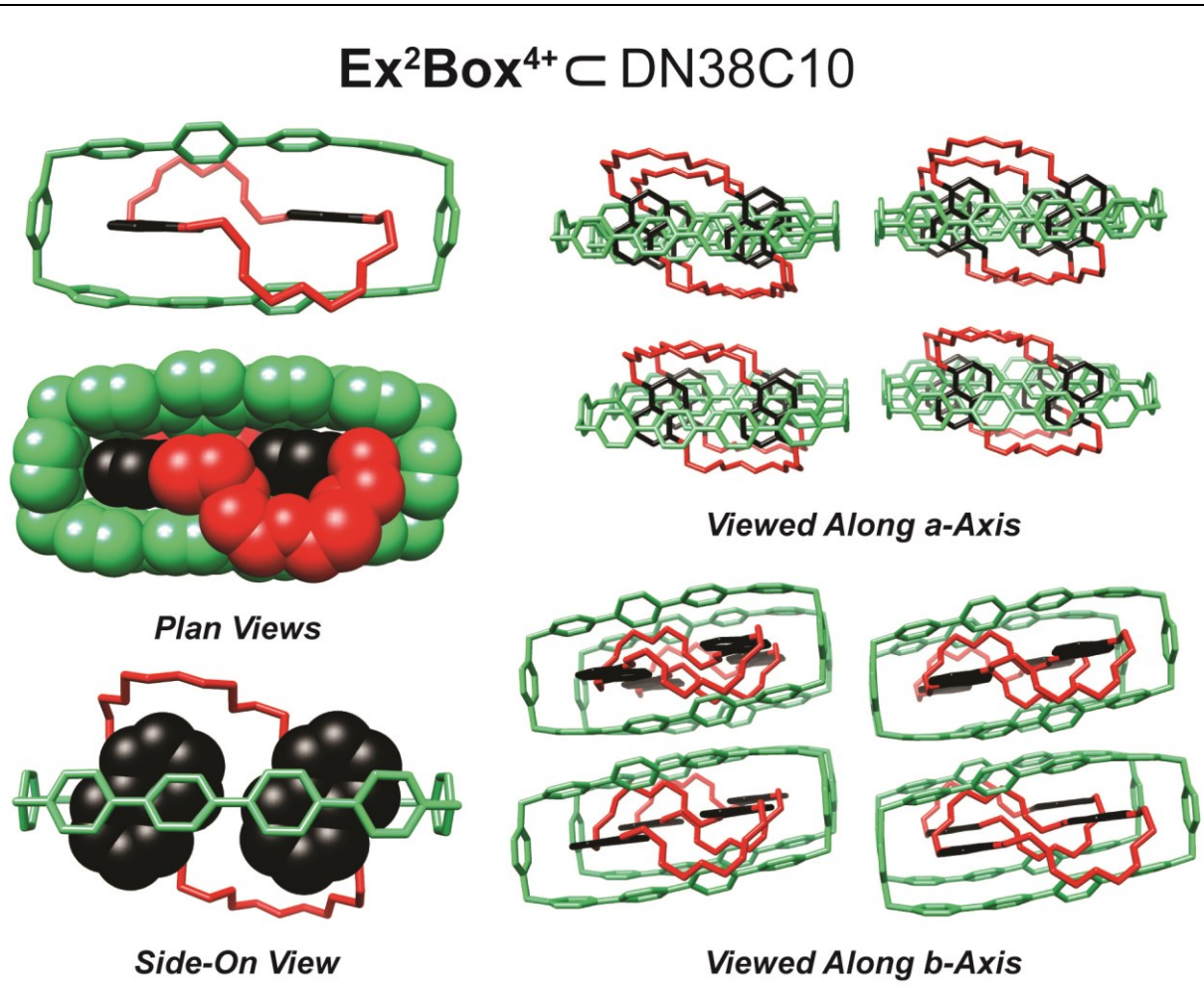


Figure S13. Different crystallographic views of **Ex²Box⁴⁺**⊂(1,5-dinaphtho[38]crown-10). Counterions and solvent molecules are omitted for the sake of clarity. DN38C10 = 1,5-dinaphtho[38]crown-10.

b) Crystal Parameters. $[C_{60}H_{48}N_4 \subset C_{36}H_{44}O_{10} \bullet (PF_6)_4] \bullet (MeCN)_8$. Orange block (0.47 × 0.13 × 0.08 mm). Triclinic, $P\bar{1}$, a = 10.821(3), b = 13.528(3), c = 21.903(6) Å, α = 88.571(13), β = 86.429(12), γ = 72.761(11)º, V = 3056.3(14) Å^3, Z = 1, T = 99.98 K, ρ_{calc} = 1.286 g cm^{-3}, μ = 1.398 mm^{-1}. Of a total of 24907 reflections that were collected, 10092 were unique. Final R_1 = 0.0562 and wR_2 = 0.1607. The enhanced rigid-bond restraint was applied[6] to the disordered atoms. Distance restraints were also refined for the disordered atoms. CCDC Number: 913424.

Section E. Spectroscopic and Spectrometric Characterizations

1) ^{1}H NMR Spectroscopic Analysis

^{1}H NMR (298 K, 600 MHz) titrations were performed by adding small volumes of a concentrated guest solution in CD_3CN or $CDCl_3$ to a solution of **Ex^{2}Box**•4PF_6 in CD_3CN. Tetramethylsilane was used as a reference. The upfield shifts of the ^{1}H resonances for β, γ, or δ protons were observed and used to determine the association constants (K_a). The K_a values were calculated using Dynafit,[7] a program that employs nonlinear least-squares regression on ligand–receptor binding data.

The binding ratio for the complex between **Ex^{2}Box**•4PF_6 and anthracene in solution was obtained from a Job plot (Figure S14) – using an average of two data sets – which was derived from chemical shifts of the δ protons of **Ex^{2}Box**•4PF_6 in mixtures of **Ex^{2}Box**•4PF_6 and anthracene in CD_3CN (containing up to 2.5% of $CDCl_3$ for the purposes of solubility) at 25 °C by using ^{1}H NMR spectroscopy. The data shows a 1:1 binding between **Ex^{2}Box**•4PF_6 and anthracene.

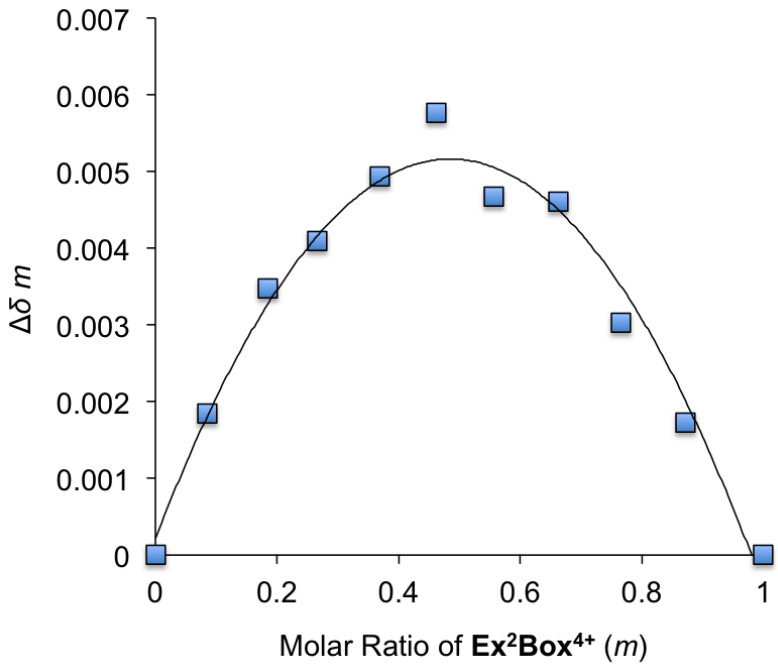


Figure S14. Job plot for the complex between **Ex^{2}Box**•4PF_6 and anthracene in CD_3CN at room temperature, showing a 1:1 binding ratio in solution.

2) Cyclic Voltammetric Analysis

Cyclic voltammetry was carried out on a 1.0 mM solution of **Ex^{2}Box**•4PF$_6$ in MeCN using 0.1 M TBAPF$_6$ as the electrolyte and a Ag/AgCl reference electrode at 298 K. The cyclic voltammogram (CV) for **Ex^{2}Box**•4PF$_6$ is displayed at the bottom of Figure S15 (green) and demonstrates a single, broad reduction and oxidation wave, which are separated by 280 mV. Comparing the CV of **Ex^{2}Box**•4PF$_6$ to the CVs of **CBPQT**•4PF$_6$ (top) and **ExBox**•4PF$_6$ (middle), it becomes evident – as the redox couples merge into one starting from **CBPQT**•4PF$_6$ and going to **Ex^{2}Box**•4PF$_6$ – that the electronic coupling (communication) decreases as the number of the phenylene rings between the pyridinium rings is increased to one (**ExBox**•4PF$_6$) and two (**Ex^{2}Box**•4PF$_6$). This decreased electronic coupling occurs as a result of the torsional twisting between each ring, which disrupts the conjugation between the redox centers.

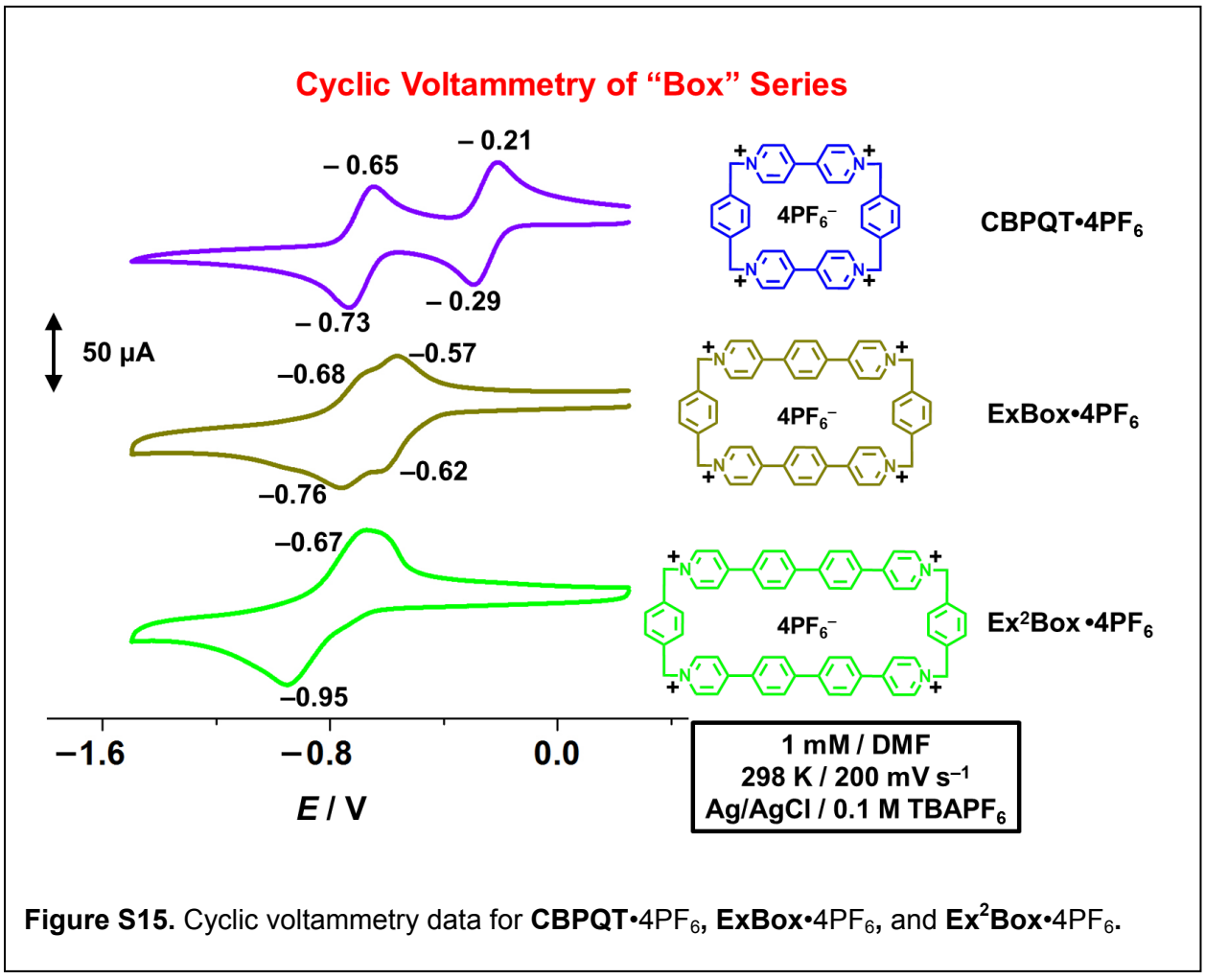


Figure S15. Cyclic voltammetry data for **CBPQT**•4PF$_6$, **ExBox**•4PF$_6$, and **Ex^{2}Box**•4PF$_6$.

3) UV/Vis Spectroscopic Analysis

The UV/Vis absorption spectra were recorded for **Ex^{2}Box**•4PF$_6$ (Figure S16) and its soluble 1:1 complexes **Ex^{2}Box**•4PF$_6$⊂guest (Figure S17), where the guests ranged from electron-rich (a) anthracene, (b) pyrene, (c) tetraphene, and (d) chrysene to electron-poor (e) 2,6-dinitrotoluene (DNT), (f) 1,5-dinitronaphthalene (DNN), (g) 9,10-anthraquinone (9,10-AQ), and (h) 1,4-anthraquinone (1,4-AQ), to (i) 1,4-bis(3-methoxyphenyl)-1*H*-1,2,3-triazole (BMPT) and (j) 1,5-dinaphtho[38]crown-10 (DN38C10) all at 0.5 mM in a 1-cm cell at 298 K. It is important to note the red-shifted charge-transfer bands in each of the electron-rich guests as a result of the charge-transfer interactions of the respective guests with **Ex^{2}Box**•4PF$_6$, while the electron-poor guests display no appreciable difference in their absorption spectra between the empty cyclophane and the mixture of the host and guest either on account of their different modes of binding or weak binding at 0.5 mM. Additionally, the UV/Vis spectrum where tetracene is the guest was not recorded because of the limited solubility.

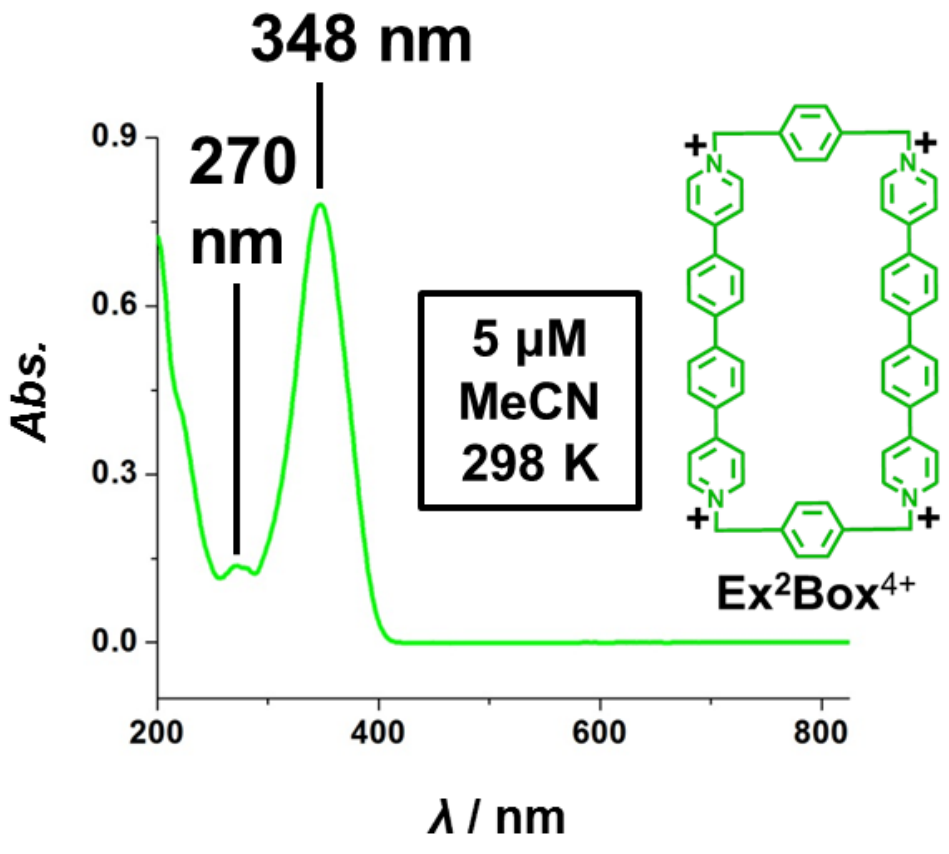


Figure S16. UV/Vis Spectra of **Ex^{2}Box**•4PF$_6$ at 0.5 mM in a 1-cm cell at 298 K.

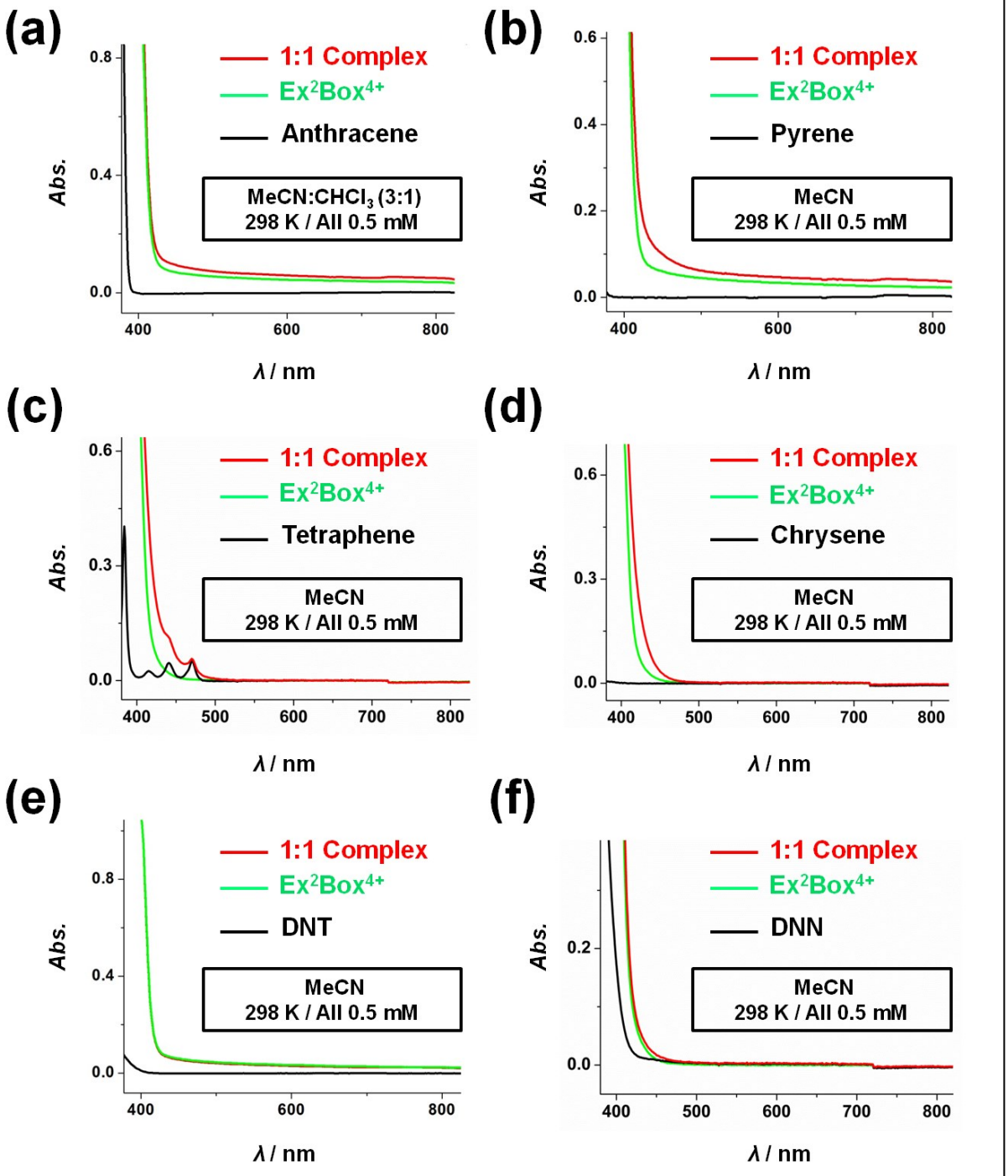


Figure S17a–f. UV/Vis Spectra of the soluble 1:1 complexes of **Ex²Box**•4PF_6⊂ guest, where the guests are (a) anthracene, (b) pyrene, (c) tetraphene, (d) chrysene, (e) DNT, and (f) DNN all at 0.5 mM in a 1-cm cell at 298 K.

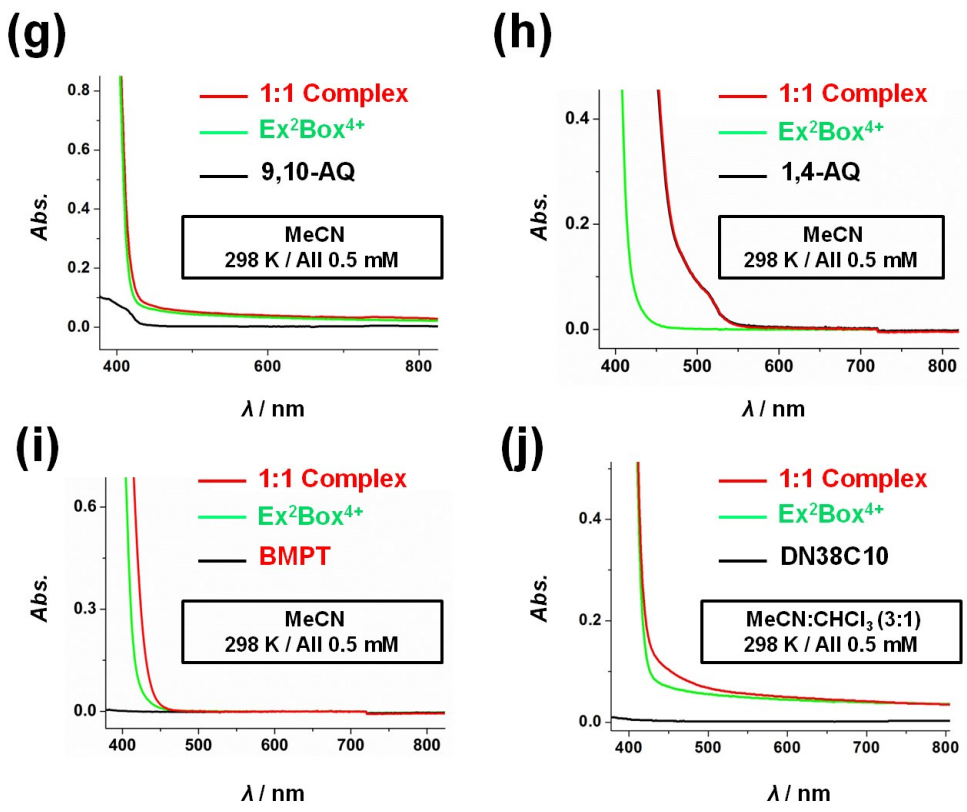


Figure S17g–j. UV/Vis Spectra of the soluble 1:1 complexes of **Ex^{2}Box**•4PF_6⊂ guest, where the guests are (g) 9,10-AQ, (h) 1,4-AQ, (i) BMPT, and (j) D38C10, all at 0.5 mM in a 1-cm cell at 298 K.

Section F. References

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